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A Theoretical Extension of the Reduced-Cell Concept in Crystallography

by

R. B. Roof, Jr.

Abstract

Special and degenerate representations for reduced cells have been derived from the 41 Niggli matricies for general reduced cells. They are combined with the representations for the general reduced cells to form an expanded classification scheme based on specific relationships between the individual elements of the matrix representation. Typographical errors in several references are noted and corrected.

1. Introduction

The purpose of this paper is to lay the foundation for a computer program to be written for indexing unknown X-ray powder patterns. The concept of a Niggli reduced cell is used; the figures upon which this type of cell is based have been redrawn to emphasize the positive direction of, and the appropriate angles between, the various vectors defining the cell. Typographical errors in several references are noted and corrected. An expansion of a classification table is made that includes special and degenerate cases of the reduced cell for which no entry to the classification table has been previously provided, and, finally, the classification table is arranged in a manner convenient for computer programming.

The concept of a reduced cell has been familiar in the field of crystallography for several decades. The reduced cell used in this paper is a special cell, a specific one of the infinite number of cells which may be used to describe or characterize a lattice. Briefly, it is <u>the unit cell having as edges the shortest three noncoplanar translations of the lattice</u>.

In addition, as outlined by Azaroff and Buerger (1958), pg. 129-131, a unit cell may be characterized by having the cosines of the interaxial angles all positive (type I) or all negative (type II). Any mixture of positive and negative cosines may be transformed to either type I or type II by appropriate reversal of the individual axial directions. Therefore, the reduced cell may be further characterized as <u>also having the interaxial angles either all acute or all obtuse</u>.

2. The Niggli matrix representation

A unit cell of a lattice is usually described by listing the three cell edges, $\underline{a}$, $\underline{b}$, $\underline{c}$, and the three interaxial angles, α, β, γ. However, the following scalar products

$$\underset{\sim}{a}\cdot\underset{\sim}{a} = \underline{a}^2 \qquad (1)$$

$$\underset{\sim}{b}\cdot\underset{\sim}{b} = \underline{b}^2 \qquad (2)$$

$$\underset{\sim}{c}\cdot\underset{\sim}{c} = \underline{c}^2 \qquad (3)$$

$$\underset{\sim}{a}\cdot\underset{\sim}{b} = \underline{ab}\cos\gamma \qquad (4)$$

$$\underset{\sim}{a}\cdot\underset{\sim}{c} = \underline{ac}\cos\beta \qquad (5)$$

$$\underset{\sim}{b}\cdot\underset{\sim}{c} = \underline{bc}\cos\alpha \qquad (6)$$

may also be taken as an exact representation of the cell, since the six quantities $\underline{a}$, $\underline{b}$, $\underline{c}$, and α, β, γ can be readily derived from them. For identification purposes the six scalar products may be arranged in a particular format, specifically a rectangular array

$$\begin{pmatrix} \underset{\sim}{a}\cdot\underset{\sim}{a} & \underset{\sim}{b}\cdot\underset{\sim}{b} & \underset{\sim}{c}\cdot\underset{\sim}{c} \\ \underset{\sim}{b}\cdot\underset{\sim}{c} & \underset{\sim}{a}\cdot\underset{\sim}{c} & \underset{\sim}{a}\cdot\underset{\sim}{b} \end{pmatrix} \qquad (7)$$

The numerical aspects of these scalar products may be emphasized by writing the rectangular array as

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ S_{23} & S_{13} & S_{12} \end{pmatrix} \qquad (8)$$

In this case S_{23} represents the scalar product between the axes labeled 2 and 3, etc. Any particular cell may be represented by setting down in the array format the numerical values of these six quantities.

Since there are 14 space lattice types it might be supposed that there are also 14 reduced-cell representations. Actually, because some lattice types have several different representations which depend in detail on the various dimensional relations and specific identification of the three axes of the unit cell, there is a total of 41 "standard" representations for all the cases of general reduced cells. These have been discussed in detail by Niggli (1928) and by Azaroff and Buerger, (1958) and are also discussed here in Appendix C. In many cases an "alternative" (as opposed to "standard") representation may be found for a general reduced cell. This "alternative" representation is just as legitimate a representation as the "standard". In order to limit the number of reduced-cell representations to be considered <u>in toto</u>, the usual convention is to assign the value -0.0 to the cosine of 90°. Thus, the "standard" representation will in general, if at all possible, be a unit cell of type II. For example, a simple orthorhombic reduced cell has three unequal edges and three angles equal to 90°. The "standard" representation thus has $\mathbf{a}\cdot\mathbf{b} = -0.0$, $\mathbf{a}\cdot\mathbf{c} = -0.0$, and $\mathbf{b}\cdot\mathbf{c} = -0.0$, whereas the "alternative" representation would have these quantities equal to +0.0.

In Niggli's treatment of general reduced-cell types the three shortest noncoplanar vectors are labeled $\mathbf{e}$, $\mathbf{f}$, $\mathbf{g}$ with $\mathbf{e} < \mathbf{f} < \mathbf{g}$. In a later section of this paper it will be shown that there exist "standard" representations in which two (or three) of the $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$ vectors are equal in magnitude and that these do not correspond to any of the 41 general reduced-cell "standard" representations. Such reduced cells are designated special or degenerate to distinguish them from a general reduced cell.

The remainder of this paper will be concerned with the following four types of representations:

1. "Standard" general representations
2. Alternative general representations
3. "Standard" degenerate representations
4. Alternative degenerate representations

For convenience the reduced-cell types discussed by Niggli have been redrawn and are given in Appendix A.

Table 1 lists the rectangular array (hereafter designated a Niggli matrix) representation of the reduced-cell types drawn in Appendix A. This table is a correction of Table 6, pg 146, of Azaroff and Buerger.

Table 1. The Niggli matrix representation of the reduced cells. (Numbers are Niggli's figure numbers.)

	P	I
Cubic	$\begin{pmatrix} s_{11} & s_{11} & s_{11} \\ \bar{\delta} & \bar{\delta} & \bar{\delta} \end{pmatrix}$ (44 A)	$\begin{pmatrix} s_{11} & s_{11} & s_{11} \\ 1/3\,\bar{s}_{11} & 1/3\,\bar{s}_{11} & 1/3\,\bar{s}_{11} \end{pmatrix}$ (44 B)
Tetragonal	$\begin{pmatrix} s_{11} & s_{11} & s_{33} \\ \bar{\delta} & \bar{\delta} & \bar{\delta} \end{pmatrix}$ (45 A)	$\begin{pmatrix} s_{11} & s_{11} & s_{33} \\ 1/2\,\bar{s}_{11} & 1/2\,\bar{s}_{11} & \bar{\delta} \end{pmatrix}$ (45 C)
	$\begin{pmatrix} s_{11} & s_{22} & s_{22} \\ \bar{\delta} & \bar{\delta} & \bar{\delta} \end{pmatrix}$ (45 B)	$\begin{pmatrix} s_{11} & s_{11} & s_{11} \\ 1/2(\bar{s}_{11} - \bar{s}_{12}) & 1/2(\bar{s}_{11} - \bar{s}_{12}) & \bar{s}_{12} \end{pmatrix}$ (45 D)
		$\begin{pmatrix} s_{11} & s_{22} & s_{22} \\ 1/4\,s_{11} & 1/2\,s_{11} & 1/2\,s_{11} \end{pmatrix}$ (45 E)
Hexagonal	$\begin{pmatrix} s_{11} & s_{11} & s_{33} \\ \bar{\delta} & \bar{\delta} & 1/2\,\bar{s}_{11} \end{pmatrix}$ (48 A)	
	$\begin{pmatrix} s_{11} & s_{22} & s_{22} \\ 1/2\,\bar{s}_{22} & \bar{\delta} & \bar{\delta} \end{pmatrix}$ (48 B)	
Orthorhombic	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \bar{\delta} & \bar{\delta} & \bar{\delta} \end{pmatrix}$ (50 C)	$\begin{pmatrix} s_{11} & s_{11} & s_{11} \\ \bar{s}_{23} & \bar{s}_{13} & (\bar{s}_{11} - \bar{s}_{23} - \bar{s}_{13}) \end{pmatrix}$ (52 A)
		$\begin{pmatrix} s_{11} & s_{22} & s_{22} \\ s_{23} & \frac{s_{11}}{2} & \frac{s_{11}}{2} \end{pmatrix}$ (52 B)
		$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \frac{\bar{s}_{22}}{2} & \frac{\bar{s}_{11}}{2} & \bar{\delta} \end{pmatrix}$ (52 C)
Monoclinic	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \bar{\delta} & \bar{s}_{13} & \bar{\delta} \end{pmatrix}$ (53 A)	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \ast 1/2(\bar{s}_{22} - \bar{s}_{12}) & \ast 1/2(\bar{s}_{11} - \bar{s}_{12}) & \bar{s}_{12} \end{pmatrix}$ (57 A)
	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \bar{s}_{23} & \bar{\delta} & \bar{\delta} \end{pmatrix}$ (53 B)	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \bar{s}_{23} & \bar{s}_{13} & (\bar{s}_{11} - \bar{s}_{23} - \bar{s}_{13}) \end{pmatrix}$ (57 B)
	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \bar{\delta} & \bar{\delta} & \bar{s}_{12} \end{pmatrix}$ (53 C)	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ s_{23} & 1/2\,s_{11} & \ast 1/2\,s_{11} \end{pmatrix}$ (57 C)
Triclinic	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ s_{23} & s_{13} & s_{12} \end{pmatrix}$ (58 A)	
	$\begin{pmatrix} s_{11} & s_{22} & s_{33} \\ \bar{s}_{23} & \bar{s}_{13} & \bar{s}_{12} \end{pmatrix}$ (58 B)	

(An * designates a corrected element in the matrix.)

F	C	R
$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ 1/2\ S_{11} & 1/2\ S_{11} & 1/2\ S_{11} \end{pmatrix}$ (44 C)		
		$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ 1/2\ S_{11} & 1/2\ S_{11} & 1/2\ S_{11} \end{pmatrix}$ (49 B) $\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ S_{23} & S_{23} & S_{23} \end{pmatrix}$ (49 C) $\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \bar{S}_{23} & \bar{S}_{23} & \bar{S}_{23} \end{pmatrix}$ (49 D) $\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ 1/2\left(\bar{S}_{22} - 1/3\ \bar{S}_{11}\right) & 1/3\ \bar{S}_{11} & 1/3\ \bar{S}_{11} \end{pmatrix}$ (49 E)
$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{S}_{23} & \bar{S}_{23} & \left(\bar{S}_{11} - 2\ \bar{S}_{23}\right) \end{pmatrix}$ (51 A) $\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ *\frac{S_{11}}{4} & *\frac{S_{11}}{2} & *\frac{S_{11}}{2} \end{pmatrix}$ (51 B)	$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & 1/2\ \bar{S}_{11} & \bar{0} \end{pmatrix}$ (50 A) $\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \bar{0} & 1/2\ \bar{S}_{11} \end{pmatrix}$ (50 B) $\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ 1/2\ \bar{S}_{22} & \bar{0} & \bar{0} \end{pmatrix}$ (50*F) $\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{0} & \bar{0} & \bar{S}_{12} \end{pmatrix}$ (50 D) $\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \bar{S}_{23} & \bar{0} & \bar{0} \end{pmatrix}$ (50 E)	
C		C
$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{S}_{23} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{pmatrix}$ (54 A) $\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{\bar{S}_{22}}{2} & \bar{S}_{13} & \bar{0} \end{pmatrix}$ (54 B) $\begin{pmatrix} *S_{11} & S_{22} & S_{33} \\ *\bar{S}_{23} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{pmatrix}$ (54 C)	$\begin{pmatrix} S_{11} & *S_{11} & S_{33} \\ *\overset{\pm}{S}_{23} & *\overset{\pm}{S}_{23} & *\overset{\pm}{S}_{12} \end{pmatrix}$ (55 A) $\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ *\overset{\pm}{S}_{23} & *\overset{\pm}{S}_{13} & *\overset{\pm}{S}_{13} \end{pmatrix}$ (55 B)	$\begin{pmatrix} S_{11} & *S_{22} & S_{33} \\ 1/2\ S_{12} & 1/2\ S_{11} & S_{12} \end{pmatrix}$ (56 A) $\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ 1/2\ S_{22} & *1/2\ S_{12} & S_{12} \end{pmatrix}$ (56 B) $\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ 1/2\ S_{13} & S_{13} & 1/2\ S_{11} \end{pmatrix}$ (56 C)

3. The transformation matrices

All reduced cells are considered to be primitive triclinic cells. Special angles, i.e. 90°, or other relationships involving symmetry of the lattices result in particular values for many of the terms in the Niggli matrix. These values and relationships form the basis for the classification system which will be described in the next section.

The axes of a reduced cell are identical with the axes of a second unit cell only if the second unit cell is itself primitive. In all other cases the axes of a second cell that has more symmetry elements than the reduced cell may be found from the axes of the reduced cell with the aid of a transformation.

In the general case this transformation has the form

$$\begin{aligned} \underline{a}_t &= U_1\underline{a}_r + V_1\underline{b}_r + W_1\underline{c}_r \\ \underline{b}_t &= U_2\underline{a}_r + V_2\underline{b}_r + W_2\underline{c}_r \\ \underline{c}_t &= U_3\underline{a}_r + V_3\underline{b}_r + W_3\underline{c}_r \end{aligned} \tag{9}$$

where $(\underline{a}, \underline{b}, \underline{c})_t$ = the axes of the transformed cell,

$(\underline{a}, \underline{b}, \underline{c})_r$ = the axes of the reduced cell

and $(U, V, W)_{1,2,3}$ = coefficients of the vector translations.

Since in specific cases only the coefficients of Eq (9) vary, the transformation process is usually represented by a matrix. For Eq (9) the matrix is

$$\begin{pmatrix} U_1 & V_1 & W_1 \\ U_2 & V_2 & W_2 \\ U_3 & V_3 & W_3 \end{pmatrix} \tag{10}$$

Different terms of the matrix (10) imply different degrees of symmetry in the transformed cell. In Table 2 are listed the transformation matrices to be used with the reduced-cell representations of Table 1. The Niggli figure numbers provide a convenient cross-correlation between Table 1 and 2. Table 2 is a correction of Table 7, pg 148, of Azaroff and Buerger.

The interaxial angles of the transformed cell may also be found by utilizing Eq (9). No transformation of interaxial angles is required in the triclinic case since the reduced cell is primitive. In all other cases the only transformed-cell interaxial angle calculation required is for angle β for monoclinic crystals. This may be computed according to the folowing analysis.

The scalar product of $\underline{a}$ and $\underline{c}$ of the transformed cell is given by

$$\underset{\sim}{a}_t \cdot \underset{\sim}{c}_t = |\underset{\sim}{a}_t| \times |\underset{\sim}{c}_t| \times \cos(\underset{\sim}{a}_t \wedge \underset{\sim}{c}_t) \qquad (11)$$

$$\therefore \cos \beta_t = \frac{\underset{\sim}{a}_t \cdot \underset{\sim}{c}_t}{\underset{\sim}{a}_t \underset{\sim}{c}_t} \qquad (12)$$

Substituting from Eq (9) for scalar product $\underset{\sim}{a}_t \cdot \underset{\sim}{c}_t$ gives

$$\cos \beta_t = \frac{1}{\underset{\sim}{a}_t \underset{\sim}{c}_t} \left\{ (U_1 \underset{\sim}{a}_r + V_1 \underset{\sim}{b}_r + W_1 \underset{\sim}{c}_r) \cdot (U_3 \underset{\sim}{a}_r + V_3 \underset{\sim}{b}_r + W_3 \underset{\sim}{c}_r) \right\} \qquad (13)$$

Table 2. Transformation matrices from reduced cells to unit cells.
(Numbers are Niggli's figure numbers.)(An * designates a corrected matrix row.)

	P	I	F	C	R
Cubic	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$ (44 A)	$\begin{pmatrix}1&0&1\\1&1&0\\0&1&1\end{pmatrix}$ (44 B)	$\begin{pmatrix}1&\bar{1}&1\\1&1&\bar{1}\\\bar{1}&1&1\end{pmatrix}$ (44 C)		
Tetragonal	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$ (45 A) $\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$ (45 B)	$\begin{pmatrix}1&0&0\\0&1&0\\1&1&2\end{pmatrix}$ (45 C) $\begin{matrix}\\ *\\ *\end{matrix}\begin{pmatrix}1&0&1\\0&1&1\\1&1&0\end{pmatrix}$ (45 D) $\begin{pmatrix}0&\bar{1}&1\\1&\bar{1}&\bar{1}\\1&0&0\end{pmatrix}$ (45 E)			
Hexagonal	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$ (48 A) $\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$ (48 B)				$\begin{pmatrix}1&0&0\\\bar{1}&1&0\\\bar{1}&\bar{1}&3\end{pmatrix}$ (49 B) $\begin{pmatrix}1&\bar{1}&0\\\bar{1}&0&1\\\bar{1}&\bar{1}&\bar{1}\end{pmatrix}$ (49 C) $\begin{pmatrix}1&\bar{1}&0\\\bar{1}&0&1\\\bar{1}&\bar{1}&\bar{1}\end{pmatrix}$ (49 D) $\begin{pmatrix}1&2&1\\0&\bar{1}&1\\1&0&0\end{pmatrix}$ (49 E)

Orthorhombic	$\begin{pmatrix}100\\010\\001\end{pmatrix}$ (50 C)	$\begin{pmatrix}101\\110\\011\end{pmatrix}$ (52 A) $\begin{pmatrix}\bar{1}00\\\bar{1}11\\0\bar{1}1\end{pmatrix}$ (52 B) $\begin{pmatrix}100\\010\\\bar{1}\bar{1}\bar{2}\end{pmatrix}$ (52 C)	$\begin{pmatrix}1\bar{1}0\\112\\\bar{1}\bar{1}0\end{pmatrix}$ (51 A) $\begin{pmatrix}\bar{1}20\\\bar{1}02\\100\end{pmatrix}$ (51 B)	$\begin{pmatrix}100\\\bar{1}0\bar{2}\\010\end{pmatrix}$ (50 A) $\begin{pmatrix}100\\\bar{1}\bar{2}0\\001\end{pmatrix}$ (50 B) $\begin{pmatrix}010\\0\bar{1}\bar{2}\\100\end{pmatrix}$ (50 F) $\begin{pmatrix}110\\\bar{1}10\\001\end{pmatrix}$ (50 D) $\begin{pmatrix}011\\0\bar{1}1\\100\end{pmatrix}$ (50 E)	
Monoclinic	$\begin{pmatrix}100\\010\\001\end{pmatrix}$ (53 A) $\begin{pmatrix}010\\100\\001\end{pmatrix}$ (53 B) $\begin{pmatrix}100\\001\\010\end{pmatrix}$ (53 C)	$\begin{pmatrix}100\\112\\011\end{pmatrix}$ (57 A) $\begin{pmatrix}011\\110\\101\end{pmatrix}$ (57 B) * $\begin{pmatrix}01\bar{1}\\100\\\bar{1}11\end{pmatrix}$ (57 C)	$\begin{pmatrix}120\\100\\001\end{pmatrix}$ (54 A) $\begin{pmatrix}012\\010\\100\end{pmatrix}$ (54 B) * $\begin{pmatrix}102\\100\\010\end{pmatrix}$ (54 C)	$\begin{pmatrix}110\\\bar{1}10\\001\end{pmatrix}$ (55 A) $\begin{pmatrix}011\\0\bar{1}1\\100\end{pmatrix}$ (55 B)	$\begin{pmatrix}\bar{1}00\\\bar{1}02\\010\end{pmatrix}$ (56 A) $\begin{pmatrix}0\bar{1}0\\0\bar{1}2\\100\end{pmatrix}$ (56 B) $\begin{pmatrix}\bar{1}00\\\bar{1}20\\001\end{pmatrix}$ (56 C)
Triclinic	$\begin{pmatrix}100\\010\\001\end{pmatrix}$ (58 A) $\begin{pmatrix}100\\010\\001\end{pmatrix}$ (58 B)				

$$= \frac{1}{\underset{\sim}{a}_t \underset{\sim}{c}_t} \Big\{ U_1 U_3 \underset{\sim}{a}_r^2 + V_1 V_3 \underset{\sim}{b}_r^2 + W_1 W_2 \underset{\sim}{c}_r^2$$

$$+ U_1 V_3 \underset{\sim}{a}_r \cdot \underset{\sim}{b}_r + U_1 W_3 \underset{\sim}{a}_r \cdot \underset{\sim}{c}_r \tag{14}$$

$$+ V_1 U_3 \underset{\sim}{b}_r \cdot \underset{\sim}{a}_r + V_1 W_3 \underset{\sim}{b}_r \cdot \underset{\sim}{c}_r$$

$$+ W_1 U_3 \underset{\sim}{c}_r \cdot \underset{\sim}{a}_r + W_1 V_3 \underset{\sim}{c}_r \cdot \underset{\sim}{b}_r \Big\}$$

Substitutions for scalar cross-product terms from Eq (4), (5), and (6) and rearrangement gives

$$\cos \beta_t = \frac{1}{\underset{\sim}{a}_t \underset{\sim}{c}_t} \Big\{ U_1 U_3 \underset{\sim}{a}_r^2 + V_1 V_3 \underset{\sim}{b}_r^2 + W_1 W_3 \underset{\sim}{c}_r^2$$

$$+ (U_1 V_3 + U_3 V_1)\ \underset{\sim}{a}_r \underset{\sim}{b}_r \cos \gamma_r \tag{15}$$

$$+ (V_1 W_3 + V_3 W_1)\ \underset{\sim}{b}_r \underset{\sim}{c}_r \cos \alpha_r$$

$$+ (W_1 U_3 + W_3 U_1)\ \underset{\sim}{c}_r \underset{\sim}{a}_r \cos \beta_r \Big\}$$

Since the cosine is known, the angle β_t may be easily found.

4. A classification system for the Niggli matrices

After the scalar array for a particular cell has been found, the next step is to identify it with one of the "standard" representations in Table 1. Niggli presented a table to perform this operation, and Azaroff and Buerger translated and rearranged this table to yield in their book Table 8, pg 150. They also describe the procedure for using their table.

Use of their procedure and Table 8, provides an elegant method of identification provided that the scalar array being examined belongs to one of the 41 "general" reduced-cell types. To realize the maximum usefulness from such a table however, one should be able to find and identify the special and degenerate cases that result when one (or two) of the reduced-cell vectors $\mathbf{e}$, $\mathbf{f}$, $\mathbf{g}$ are equal in magnitude and do not yield a representation identical with any of the "standard" 41 representations.

For example, the representation for a hexagonal cell with $c/a > 1.0$ is

$$\begin{array}{ccc} S_{11} & S_{11} & S_{33} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{array}$$

and for $c/a < 1.0$

$$\begin{array}{ccc} S_{11} & S_{22} & S_{22} \\ \frac{\bar{S}_{22}}{2} & \bar{0} & \bar{0} \end{array}$$

Both of these representations are in the table. But for $c/a = 1.0$, the representation for a hexagonal cell may be

$$\begin{array}{ccc} S_{11} & S_{11} & S_{11} \\ \frac{\bar{S}_{11}}{2} & \bar{0} & \bar{0} \end{array}, \text{ or } \begin{array}{ccc} S_{11} & S_{11} & S_{11} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{array}, \text{ or } \begin{array}{ccc} S_{11} & S_{11} & S_{11} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{array}$$

These three representations for the case of $c/a = 1.0$ result because it is not known which of the three identical axes is used or chosen as the "a, b, or c" axes of the unit cell. If these special representations are included in a classification scheme, then a routine search of the tables and application of the appropriate transformation matrix will result in a transformed cell having the conventional setting of $\alpha = 90°$, $\beta = 90°$, $\gamma = 120°$. Since a computer, or a human being for that matter, may find any of the three representations, a classification scheme should consider cases of this type. Azaroff and Buerger's current version of Table 8 does not allow this to be done.

All the special and degenerate cases are determined by allowing the $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$ vectors of the 41 general Niggli reduced cells to be equal to each other according to the scheme illustrated in Figure 1. Starting with the general set of vectors $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$, the vector $\underset{\sim}{g}$ may decrease in magnitude until it exactly equals the magnitude of $\underset{\sim}{f}$, then the vector set will be $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{f}$. This set may degenerate in one of two ways depending on whether the $\underset{\sim}{f}$ vector in the second or third position degenerates to equal in magnitude an $\underset{\sim}{e}$ vector. If the second vector degenerates, the set is $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{f}$. If the third vector degenerates, the set is ($\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{e}$), which, if the convention of listing the shortest vectors first is followed, transforms to $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{f}$. Extreme care must be exercised at this stage as the transformed set may or may not identically equal the $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{f}$ set obtained when the second vector of $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$ degenerates to $\underset{\sim}{e}$. Both the $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{f}$ and the ($\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{e}$) vector sets may reduce to $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{e}$ if $\underset{\sim}{f}$ degenerates to equal in magnitude the vector $\underset{\sim}{e}$.

The vector set $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$ may also degenerate in two other ways. The vector $\underset{\sim}{f}$ may go directly to an $\underset{\sim}{e}$ value; in that case $\underset{\sim}{g}$ becomes the second longest vector, which is usually designated $\underset{\sim}{f}$. Or, the original vector $\underset{\sim}{g}$ may go directly to an $\underset{\sim}{e}$ value, and in that case the representation is ($\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{e}$). This set was discussed in the previous paragraph.

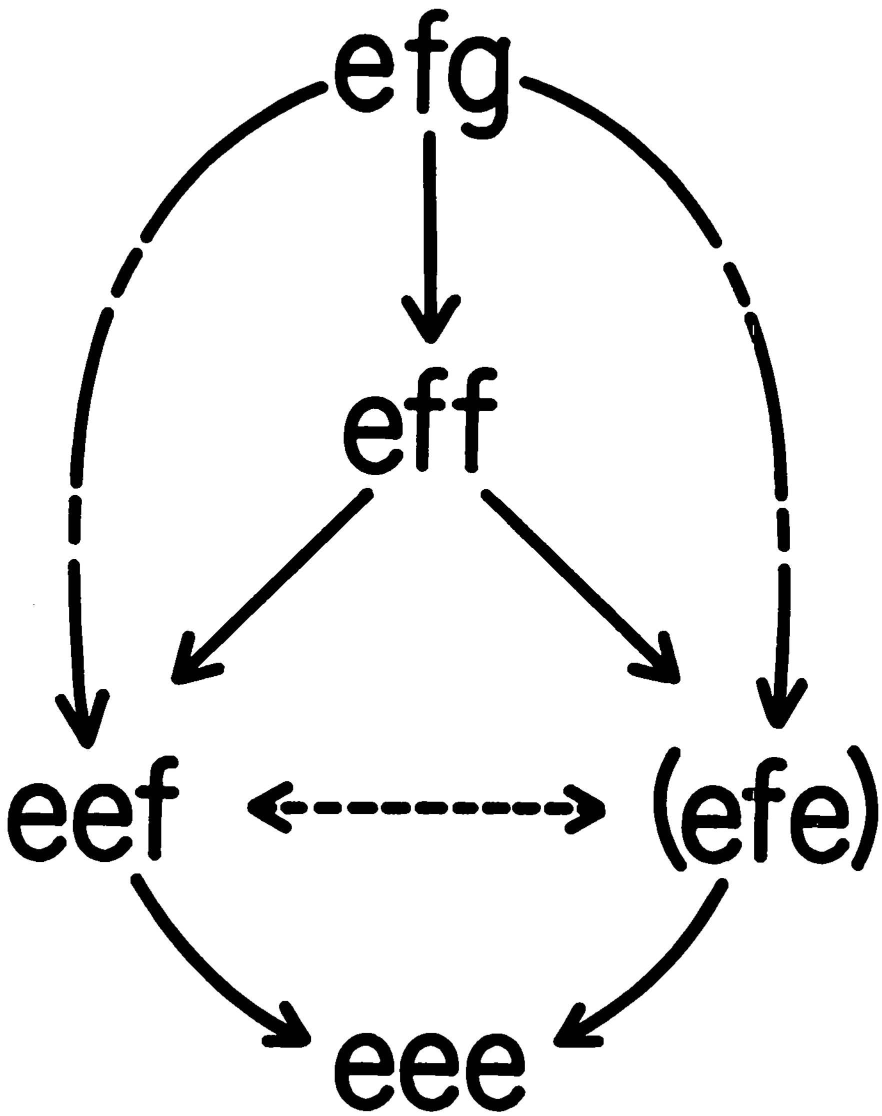

Figure 1. Flow chart for the degeneracy of three general vectors $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$ to three identical vectors $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{e}$.

If at any time during the application of Figure 1 to each of the 41 reduced cells a representation is obtained which is different from one of the 41 representations, then this representation is retained for inclusion in an expansion of the scheme of Table 8 of Azaroff and Buerger. If a representation is obtained that is equal to one of the 41 general representations, then the representation is ignored as it is adequately covered under the general headings.

An illustrative example of the derivation of special and degenerate cases is given below by applying Figure 1 to an end-centered orthorhombic cell, Niggli Figure 50A.

For 50A, $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{g}$, the reduced-cell representation is

$$\begin{matrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{matrix}$$

For 50A, $\underset{\sim}{e}$, $\underset{\sim}{f}$, $\underset{\sim}{f}$, the reduced-cell representation is

$$\begin{matrix} S_{11} & S_{22} & S_{22} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{matrix} \quad \text{or} \quad \begin{matrix} S_{11} & S_{22} & S_{22} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{matrix}$$

For 50A, $\underset{\sim}{e}$, $\underset{\sim}{e}$, $\underset{\sim}{f}$, the reduced-cell representation is

$$\begin{matrix} S_{11} & S_{11} & S_{22} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{matrix} \quad \text{or} \quad \begin{matrix} S_{11} & S_{11} & S_{22} \\ \frac{\bar{S}_{11}}{2} & \bar{0} & \bar{0} \end{matrix}$$

For 50A, (e, f, e) the reduced-cell representation is

$$\begin{array}{ccc} S_{11} & S_{22} & S_{11} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{array}$$

However, transforming to the convention of listing the shortest vectors first gives

$$\begin{array}{ccc} S_{11} & S_{11} & S_{22} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{array}$$

which is the representation for a hexagonal cell with $c/a > 1.0$.

For 50A, e, e, e, the reduced-cell representation is

$$\begin{array}{ccc} S_{11} & S_{11} & S_{11} \\ \frac{\bar{S}_{11}}{2} & \bar{0} & \bar{0} \end{array}, \text{ or } \begin{array}{ccc} S_{11} & S_{11} & S_{11} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{array}, \text{ or } \begin{array}{ccc} S_{11} & S_{11} & S_{11} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{array}$$

which is the representation for a hexagonal cell with $c/a = 1.0$.

Assuming that the hexagonal degeneracies have been previously determined, the allowable reduced magnitudes of the various vectors in 50A yield four representations that had not been seen before. Two for the e, f, f case and two for the e, e, f case. It is of special interest to note that the e, e, f case does not equal the (e, f, e) case, which illustrates the point made previously that these cases are not automatically equal.

Ninety-one special and degenerate cases were derived in this manner. These are incorporated with the standard 41 representations in

Appendix B which is an expanded version of Azaroff and Buerger's Table 8.

The use of Appendix B for identification of a reduced cell is very similar to the procedure for use with Table 8 of Azaroff and Buerger. The given scalar matrix is examined, and the table is entered under the major catagory of the symmetrical scalars being either

$$S_{11} = S_{22} = S_{33}$$

$$\text{or } S_{11} = S_{22} \neq S_{33}$$

$$\text{or } S_{11} \neq S_{22} = S_{33}$$

$$\text{or } S_{11} \neq S_{22} \neq S_{33}$$

and the minor branch of unsymmetrical scalars being either all-positive or all-negative. A quick glance down the first column of the minor branch (assume $S_{11} = S_{22} = S_{33}$ and the all-negative minor branch) identifies the unsymmetrical scalar S_{23} at some point as either $\bar{0}$, $\frac{\bar{S}_{11}}{3}$, $\frac{\bar{S}_{11}}{2}$, some other specialized value, or a general value. At that point the second column is entered to identify the scalar S_{13}. Upon identification of S_{13}, searching is transferred to the third column where special or general values are noted for the scalar S_{12}. When complete identification of the unsymmetrical scalars is achieved the table is read horizontally to determine the lattice to which the reduced cell belongs; the Niggli figure from which it was derived; and whether the figure is a standard representation, an alternative representation of the standard, or a degenerate development. Also given is the transformation matrix for converting the reduced cell to one of higher symmetry according to Eq (9) and any pertinent comments that may help to classify the transformed cell.

If a match of unsymmetrical scalars cannot be found in searching a minor branch of the table, then exit is made from the table with the knowledge that a triclinic cell is under investigation.

5. Acknowledgement

The author is indebted to Professor M. J. Buerger for helpful correspondence during the course of this work.

References

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2. Eisenstein, G., Tabelle der reducirten positive ternären quadratischen Formen. Journal für Math., vol. 41 (1851), 141-190.

3. Jones, B. W. A Table of Eisenstein-reduced positive ternary quadratic forms of determinant $\leqq$ 200. National Research Council Bulletin number 97 (1935).

4. Niggli, P. Kristallographische und strukturtheoretische Grundbegriffe, Handbuch der Experimentalphysik 7, Teil 1 (Akademische Verlagsgesellschaft, Leipzig, 1928) 108-176.

Additional Literature of Interest

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2. Buerger, M. J., Note on reduced cells, Z. Krist. 113 (1960), 52-56.

3. Dickson, L. E., Studies in the Theory of Numbers, University of Chicago Press, 1930, Chap. XI.

4. Jones, B. W., The Arithmetic theory of quadratic forms, The Carus Mathematical Monographs, Number 10, John Wiley & Sons, 1950.

Appendix A.

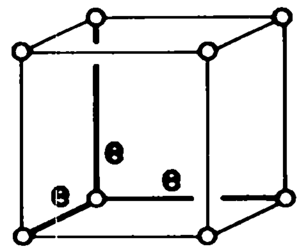
The 41 general reduced cells according to Niggli. The original figure numbers have been retained, but the relative orientations of several of the reduced cells have been changed for clarity.

(The symbol d stands for the diagonal of either a unit cell or a unit cell face depending on the context of the appropriate Niggli figure.)

A

Simple

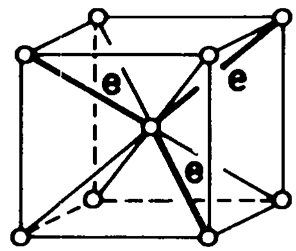
$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \bar{0} & \bar{0} & \bar{0} \end{pmatrix}$$



B

Body-centered

$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \frac{\bar{S}_{11}}{3} & \frac{\bar{S}_{11}}{3} & \frac{\bar{S}_{11}}{3} \end{pmatrix}$$



C

Face-centered

$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \frac{S_{11}}{2} & \frac{S_{11}}{2} & \frac{S_{11}}{2} \end{pmatrix}$$

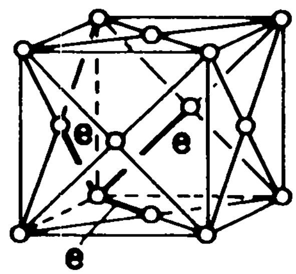


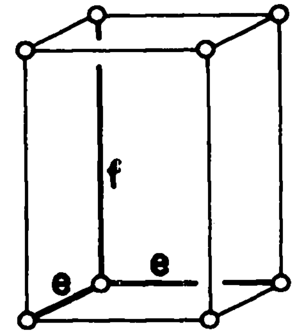
Figure 44. The three cubic lattices

A

Simple +

$a < c$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{0} & \bar{0} & \bar{0} \end{pmatrix}$$

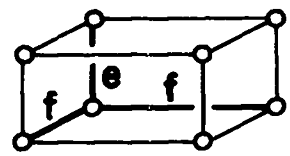


B

Simple -

$a > c$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \bar{0} & \bar{0} & \bar{0} \end{pmatrix}$$



C

Body-centered +

$\frac{c}{a} > \sqrt{2}$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \frac{\bar{S}_{11}}{2} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{pmatrix}$$

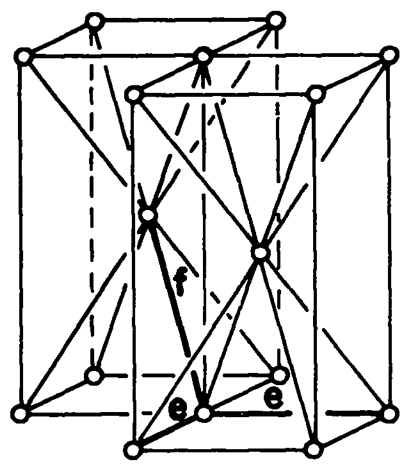


Figure 45. The five tetragonal lattices

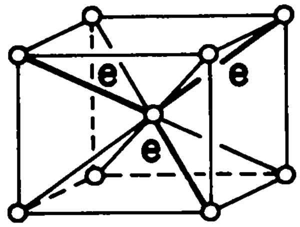
D

Body-centered

intermediate

$\sqrt{\frac{2}{3}} < \frac{c}{a} < \sqrt{2}$

$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \frac{\bar{S}_{11} - \bar{S}_{12}}{2} & \frac{\bar{S}_{11} - \bar{S}_{12}}{2} & \bar{S}_{12} \end{pmatrix}$$



E

Body-centered -

$\frac{c}{a} < \sqrt{\frac{2}{3}}$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \frac{S_{11}}{4} & \frac{S_{11}}{2} & \frac{S_{11}}{2} \end{pmatrix}$$

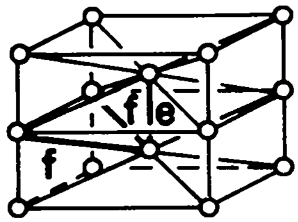


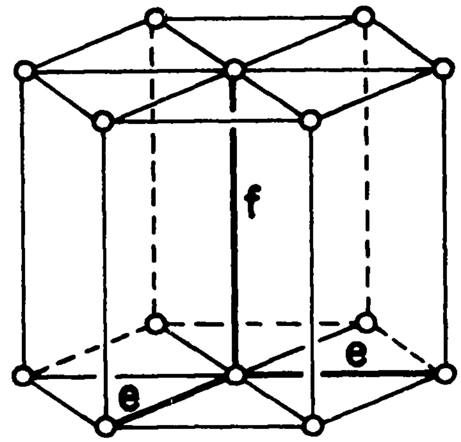
Figure 45 (cont.) The five tetragonal lattices

A

Simple +

$a < c$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{pmatrix}$$



B

Simple -

$a > c$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \frac{\bar{S}_{22}}{2} & \bar{0} & \bar{0} \end{pmatrix}$$

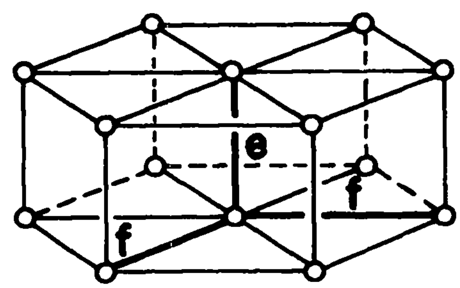


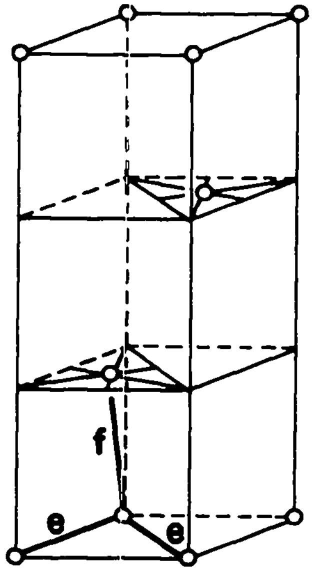
Figure 48. The two hexagonal lattices

B

Simple +

$\alpha < 60°$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \frac{S_{11}}{2} & \frac{S_{11}}{2} & \frac{S_{11}}{2} \end{pmatrix}$$



C

Intermediate +

$60° < \alpha < 90°$

$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ S_{23} & S_{23} & S_{23} \end{pmatrix}$$

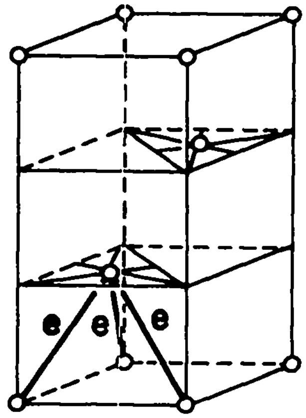


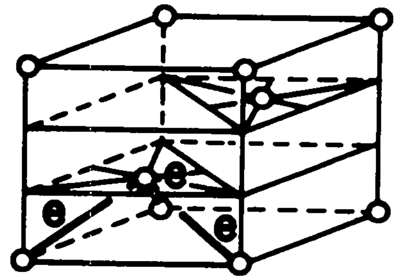
Figure 49. The four rhombohedral lattices. (Drawings are the hexagonal lattice representation)

D

Intermediate -

$90° < \alpha < 109° \; 28' \; 16.4''$

$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \bar{S}_{23} & \bar{S}_{23} & \bar{S}_{23} \end{pmatrix}$$



E

Simple -

$109° \; 28' \; 16.4'' < \alpha < 180°$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \dfrac{\bar{S}_{22} - \dfrac{\bar{S}_{11}}{3}}{2} & \dfrac{\bar{S}_{11}}{3} & \dfrac{\bar{S}_{11}}{3} \end{pmatrix}$$

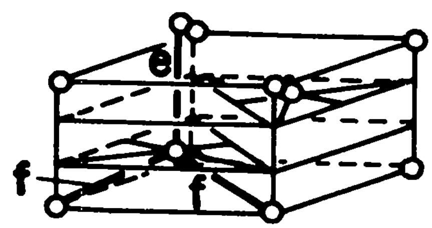


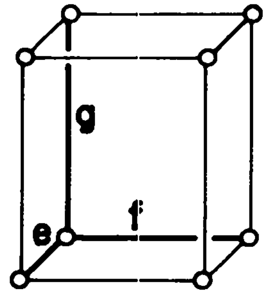
Figure 49. (cont.) The four rhombohedral lattices

C

Simple

$a^2 < b^2 < c^2$

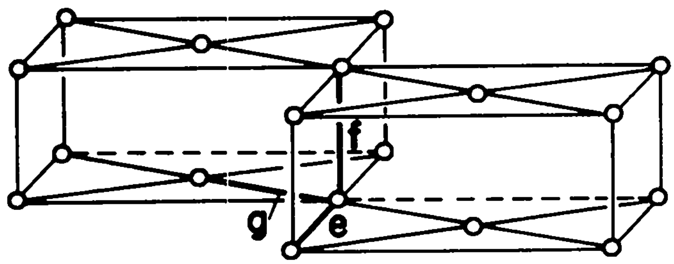
$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \bar{0} & \bar{0} \end{pmatrix}$$



A

$a^2 < c^2 < \frac{d^2}{4}$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{pmatrix}$$



B

$a^2 < \frac{d^2}{4} < c^2$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{pmatrix}$$

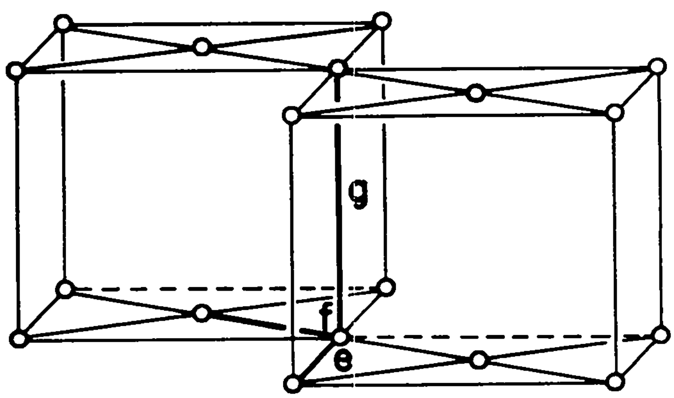


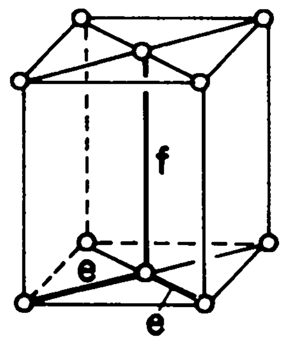
Figure 50. Simple Orthorhombic and five C-centered Orthorhombic lattices.

D

$$\frac{d^2}{4} < a^2$$

$$\frac{d^2}{4} < c^2$$

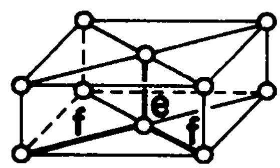
$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{0} & \bar{0} & \bar{S}_{12} \end{pmatrix}$$



E

$$c^2 < \frac{d^2}{4} < a^2$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \bar{S}_{23} & \bar{0} & \bar{0} \end{pmatrix}$$



F

$$c^2 < a^2 < \frac{d^2}{4}$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{\bar{S}_{22}}{2} & \bar{0} & \bar{0} \end{pmatrix}$$

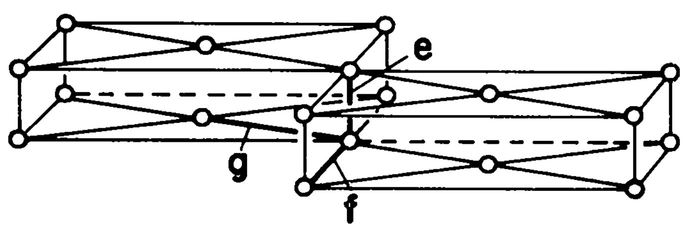
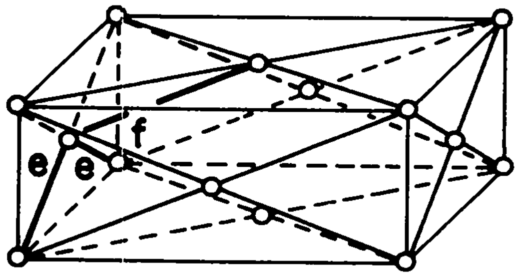


Figure 50. (cont.) Simple Orthorhombic and Five C-centered Orthorhombic Lattices

A

$$a^2 < 3\,c^2$$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{S}_{23} & \bar{S}_{23} & \left(\bar{S}_{11} - 2\,\bar{S}_{23}\right) \end{pmatrix}$$



B

$$a^2 > 3\,c^2$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{S_{11}}{4} & \frac{S_{11}}{2} & \frac{S_{11}}{2} \end{pmatrix}$$

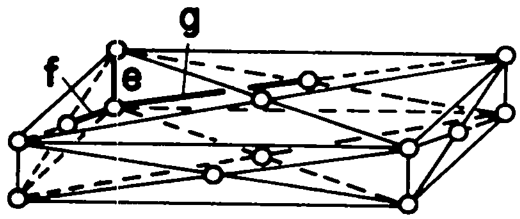
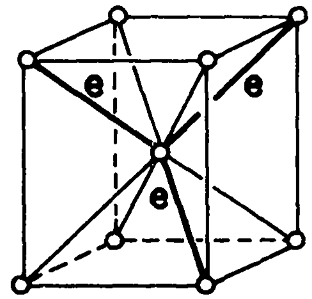


Figure 51. The two face-centered orthorhombic lattices.

A

$a < b < c$

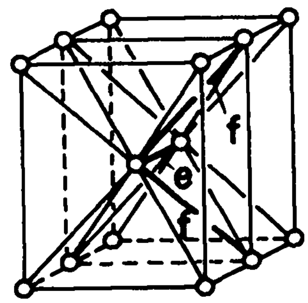
$$\begin{pmatrix} S_{11} & S_{11} & S_{11} \\ \bar{S}_{23} & \bar{S}_{13} & \left(\bar{S}_{11} - \bar{S}_{23} - \bar{S}_{13}\right) \end{pmatrix}$$



B

$a < \frac{d}{2}$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ S_{23} & \frac{S_{11}}{2} & \frac{S_{11}}{2} \end{pmatrix}$$



C

$a < b < \frac{d}{2}$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{\bar{S}_{22}}{2} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{pmatrix}$$

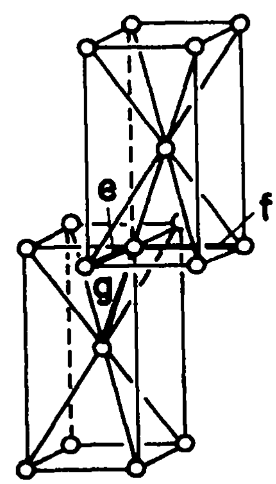
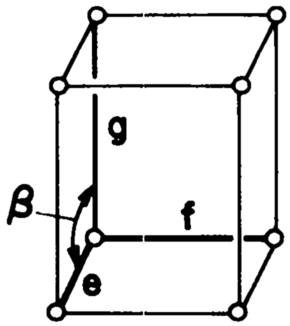


Figure 52. The three body-centered orthorhombic lattices. (See Notes 1, 2, 3, Appendix B)

A

a < b < c

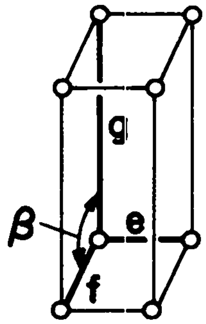
$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \bar{S}_{13} & \bar{0} \end{pmatrix}$$



B

b < a < c

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{S}_{23} & \bar{0} & \bar{0} \end{pmatrix}$$



C

a < c < b

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{0} & \bar{0} & \bar{S}_{12} \end{pmatrix}$$

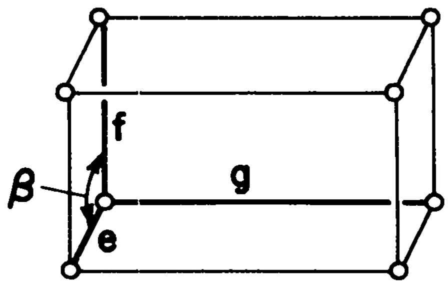
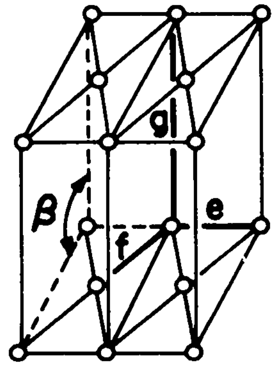


Figure 53. The three simple monoclinic lattices.

A

$$a < \frac{d}{2} < c$$

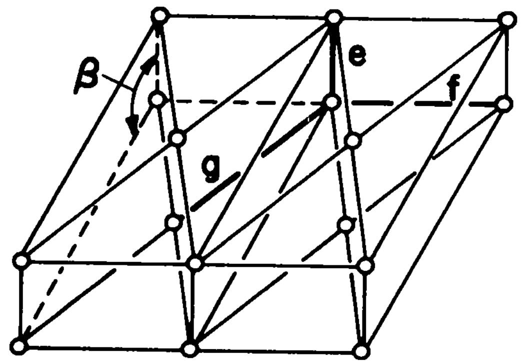
$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{S}_{23} & \bar{0} & \frac{\bar{S}_{11}}{2} \end{pmatrix}$$



B

$$c < b < \frac{d}{2}$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{\bar{S}_{22}}{2} & \bar{S}_{13} & \bar{0} \end{pmatrix}$$



C

$$b < c < \frac{d}{2}$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{S}_{23} & \frac{\bar{S}_{11}}{2} & \bar{0} \end{pmatrix}$$

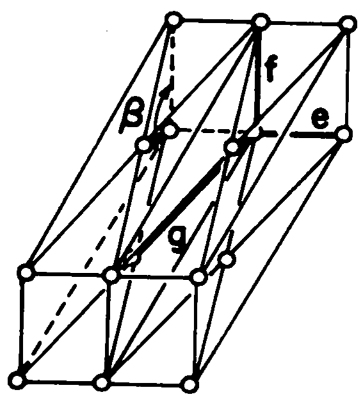
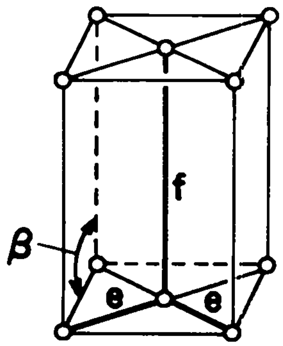


Figure 54. Three monoclinic, double primitive lattices. Two of the three primitive translations have a 90° included angle.

A

$$\frac{d}{2} < c$$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \pm & \pm & \pm \\ S_{23} & S_{23} & S_{12} \end{pmatrix}$$



B

$$c < \frac{d}{2}$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{22} \\ \pm & \pm & \pm \\ S_{23} & S_{13} & S_{13} \end{pmatrix}$$

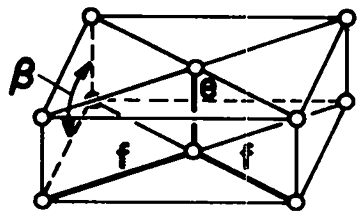
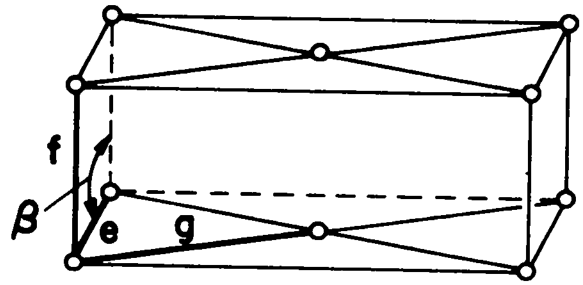


Figure 55. Two monoclinic, double primitive lattices. Two of the three primitive translations are equal, and make equal angles with the third translation.

A

$a < c < \frac{d}{2}$

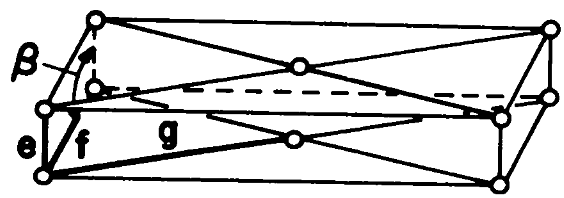
$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{S_{12}}{2} & \frac{S_{11}}{2} & S_{12} \end{pmatrix}$$



B

$c < a < \frac{d}{2}$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{S_{22}}{2} & \frac{S_{12}}{2} & S_{12} \end{pmatrix}$$



C

$a < \frac{d}{2} < c$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{S_{13}}{2} & S_{13} & \frac{S_{11}}{2} \end{pmatrix}$$

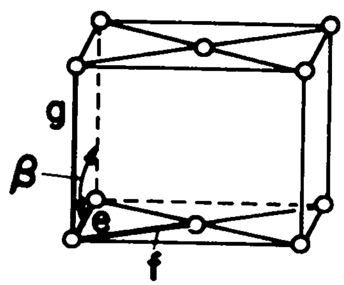
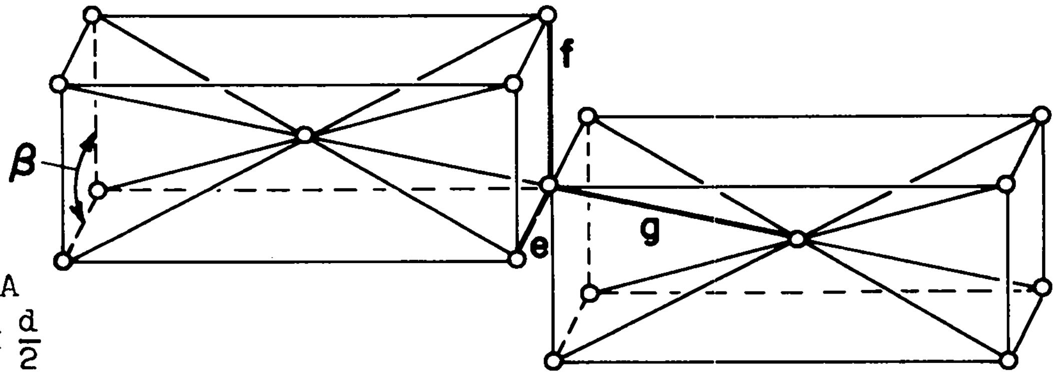


Figure 56. Three monoclinic, double primitive lattices. Two of the three primitive translations lie in the symmetry plane.



A

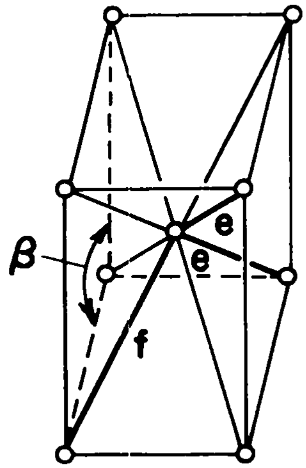
$$a < c < \frac{d}{2}$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \frac{\bar{S}_{22} - \bar{S}_{12}}{2} & \frac{\bar{S}_{11} - \bar{S}_{12}}{2} & \bar{S}_{12} \end{pmatrix}$$

B

$$\frac{d_1}{2} < \frac{d_2}{2}$$

$$\begin{pmatrix} S_{11} & S_{11} & S_{33} \\ \bar{S}_{23} & \bar{S}_{13} & \left(\bar{S}_{11} - \bar{S}_{23} - \bar{S}_{13}\right) \end{pmatrix}$$



C

$$b < \frac{d_1}{2} < \frac{d_2}{2}$$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ S_{23} & \frac{S_{11}}{2} & \frac{S_{11}}{2} \end{pmatrix}$$

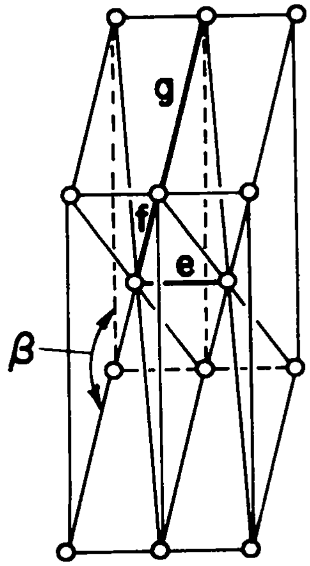
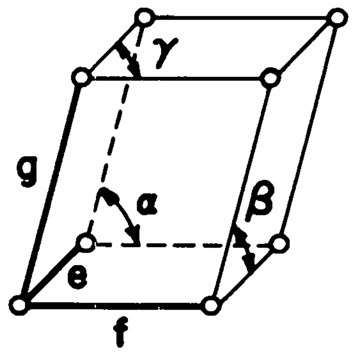


Figure 57. Three body-centered monoclinic lattices.

A

$a < b < c$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ S_{23} & S_{13} & S_{12} \end{pmatrix}$$



B

$a < b < c$

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ \bar{S}_{23} & \bar{S}_{13} & \bar{S}_{12} \end{pmatrix}$$

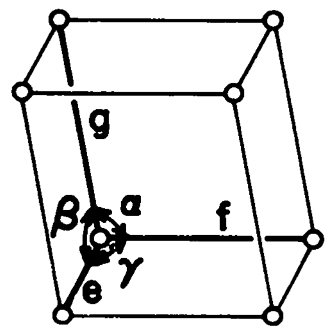


Figure 58. Two triclinic lattices

Appendix B.

Determination of reduced cell type by classification of symmetrical and unsymmetrical scalars. Special and degenerate representations derived from the 41 original Niggli reduced-cell representations are included.

(The symbol d stands for the diagonal of either a unit cell or a unit cell face depending on the context of the appropriate Niggli figure.)

Symmetrical Scalars: $S_{11} = S_{22} = S_{33}$

Unsymmetrical Scalars: +	Lattice	Niggli Figure	Transformation Matrix	Comments
$0 \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{2}$	Orthorhombic	52 B deg	$0\bar{1}\bar{1}$ $01\bar{1}$ $2\bar{1}\bar{1}$	Transformation matrix yields FCC alternative representation. See Note 3
$0 \quad S_{13} \quad S_{13}$	Monoclinic	55 A deg	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c \quad a = b$
$\frac{S_{11}}{4} \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{2}$	Tetragonal	45 E deg	$0\bar{1}1$ $1\bar{1}\bar{1}$ 100	Body-centered $\frac{c}{a} = \sqrt{\frac{2}{3}}$
$\frac{S_{11}}{2} \quad 0 \quad \frac{S_{11}}{2}$	Orthorhombic	52 B deg	$\bar{1}0\bar{1}$ $10\bar{1}$ $\bar{1}2\bar{1}$	Transformation matrix yields FCC alternative representation. See Note 3
$\frac{S_{11}}{2} \quad \frac{S_{11}}{4} \quad \frac{S_{11}}{2}$	Tetragonal	45 E deg	$\bar{1}01$ $\bar{1}1\bar{1}$ 010	Body-centered $\frac{c}{a} = \sqrt{\frac{2}{3}}$
$\frac{S_{11}}{2} \quad \frac{S_{11}}{2} \quad 0$	Orthorhombic	52 B deg	$\bar{1}\bar{1}0$ $1\bar{1}0$ $\bar{1}\bar{1}2$	Transformation matrix yields FCC alternative representation. See Note 3
$\frac{S_{11}}{2} \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{4}$	Tetragonal	45 E deg	$\bar{1}10$ $\bar{1}\bar{1}1$ 001	Body-centered $\frac{c}{a} = \sqrt{\frac{2}{3}}$
$\frac{S_{11}}{2} \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{2}$	Isometric	44 C std	$1\bar{1}1$ $11\bar{1}$ $\bar{1}11$	Face-centered cubic

$\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$ S_{12}	Orthorhombic	52 B deg	$00\bar{1}$ $11\bar{1}$ $\bar{1}10$	Body-centered $a^2 = \frac{d^2}{4} < b^2 < c^2$ See Note 3
$\frac{S_{11}}{2}$ $\frac{S_{12}}{2}$ S_{12}	Monoclinic	56 A deg	$0\bar{1}0$ $0\bar{1}2$ 100	End-centered $a^2 = c^2 = \frac{d^2}{4}$
$\frac{S_{11}}{2}$ S_{13} $\frac{S_{11}}{2}$	Orthorhombic	52 B deg	$0\bar{1}0$ $1\bar{1}1$ $\bar{1}01$	Body-centered $a^2 = \frac{d^2}{4} < b^2 < c^2$ See Note 3
$\frac{S_{11}}{2}$ S_{13} $\frac{S_{13}}{2}$	Monoclinic	56 A deg	$00\bar{1}$ $02\bar{1}$ 100	End-centered $a^2 = c^2 = \frac{d^2}{4}$
$\frac{S_{13}}{2}$ S_{13} $\frac{S_{11}}{2}$	Monoclinic	56 A deg	$\bar{1}00$ $\bar{1}20$ 001	End-centered $a^2 = c^2 = \frac{d^2}{4}$
$\frac{S_{12}}{2}$ $\frac{S_{11}}{2}$ S_{12}	Monoclinic	56 A deg	$\bar{1}00$ $\bar{1}02$ 010	End-centered $a^2 = c^2 = \frac{d^2}{4}$
S_{23} 0 S_{23}	Monoclinic	55 A deg	101 $\bar{1}01$ 010	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$ $a = b$
S_{23} $\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$	Orthorhombic	52 B deg	$\bar{1}00$ $\bar{1}11$ $0\bar{1}1$	Body-centered $a^2 = \frac{d^2}{4} < b^2 < c^2$ See Note 3
S_{23} $\frac{S_{11}}{2}$ $\frac{S_{23}}{2}$	Monoclinic	56 A deg	$00\bar{1}$ $20\bar{1}$ 010	End-centered $a^2 = c^2 = \frac{d^2}{4}$

S_{23} $\frac{S_{23}}{2}$ $\frac{S_{11}}{2}$	Monoclinic	56 A deg	$0\bar{1}0$ $2\bar{1}0$ 001	End-centered $a^2 = c^2 = \frac{d^2}{4}$
S_{23} S_{23} 0	Monoclinic	55 A deg	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c \quad a = b$
S_{23} S_{23} S_{12}	Monoclinic	55 A deg	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$
S_{23} S_{13} S_{13}	Monoclinic	55 A deg	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$
S_{23} S_{13} S_{23}	Monoclinic	55 A deg	101 $\bar{1}01$ 010	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$
S_{23} S_{23} S_{23}	Rhombohedral	49 C std	$1\bar{1}0$ $\bar{1}01$ $\overline{111}$	Transformation matrix results in a hexagonal lattice. $0.0 < \cos \alpha_r < 0.5$

Symmetrical Scalars: $S_{11} = S_{22} = S_{33}$

Unsymmetrical Scalars: -	Lattice	Niggli Figure	Transformation Matrix	Comments
$\bar{0}\ \bar{0}\ \bar{0}$	Isometric	44 A std	100 010 001	Simple Cubic
$\bar{0}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Hexagonal	48 A-B deg	100 010 001	$\frac{c}{a} = 1.0$
$\bar{0}\ \bar{0}\ \bar{S}_{12}$	Orthorhombic	50 D deg	110 $\bar{1}$10 001	C - centered $\frac{d^2}{4} < a^2; \frac{d^2}{4} = c^2$
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Hexagonal	48 A-B deg	001 100 010	$\frac{c}{a} = 1.0$
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \frac{\bar{S}_{11}}{2}$	Tetragonal	45 C deg	001 010 211	Tetragonal Representation of Face-centered Cubic
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \bar{S}_{12}$	Monoclinic	54 A deg	201 001 010	End-centered $b^2 = c^2 = \frac{d^2}{4}$
$\bar{0}\ \bar{S}_{13}\ \bar{0}$	Orthorhombic	50 D deg	101 $\bar{1}$01 010	C - centered $\frac{d^2}{4} < a^2; \frac{d^2}{4} = c^2$
$\bar{0}\ \bar{S}_{13}\ \frac{\bar{S}_{11}}{2}$	Monoclinic	54 A deg	210 010 001	End-centered $b^2 = c^2 = \frac{d^2}{4}$

$\bar{0}$ $\bar{S}_{13}$ $\bar{S}_{13}$	Monoclinic	55 A deg	011 $0\bar{1}\bar{1}$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c \quad a = b$
$\frac{\bar{S}_{11}}{3}$ $\frac{\bar{S}_{11}}{3}$, $\frac{\bar{S}_{11}}{3}$	Isometric	44 B std	101 110 011	Body-centered Cubic
$\frac{\bar{S}_{11}}{2}$ $\bar{0}$ $\bar{0}$	Hexagonal	48 A-B deg	010 001 100	$\frac{c}{a} = 1.0$
$\frac{\bar{S}_{11}}{2}$ $\bar{0}$ $\frac{\bar{S}_{11}}{2}$	Tetragonal	45 C deg	100 001 121	Tetragonal Representation of Face-centered Cubic
$\frac{\bar{S}_{11}}{2}$ $\bar{0}$ $\bar{S}_{12}$	Monoclinic	54 A deg	021 001 100	End-centered $b^2 = c^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{11}}{2}$ $\frac{\bar{S}_{11}}{2}$ $\bar{0}$	Tetragonal	45 C deg	100 010 112	Tetragonal Representation of Face-centered Cubic
$\frac{\bar{S}_{11}}{2}$ $\frac{\bar{S}_{11}}{2}$ $\bar{S}_{12}$	Orthorhombic	52 B deg	001 111 $\bar{1}10$	Body-centered $a^2 = \frac{d^2}{4} < b^2 < c^2$ See Note 3
$\frac{\bar{S}_{11}}{2}$ $\bar{S}_{13}$ $\bar{0}$	Monoclinic	54 A deg	012 010 100	End-centered $b^2 = c^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{11}}{2}$ $\bar{S}_{13}$ $\frac{\bar{S}_{11}}{2}$	Orthorhombic	52 B deg	010 111 $\bar{1}01$	Body-centered $a^2 = \frac{d^2}{4} < b^2 < c^2$ See Note 3

$\frac{\bar{S}_{11} - \bar{S}_{12}}{2}$ $\frac{\bar{S}_{11} - \bar{S}_{12}}{2}$ $\bar{S}_{12}$	Tetragonal	45 D std	101 011 110	Body-centered $\sqrt{\frac{2}{3}} \le \frac{c}{a} < \sqrt{2}$
$\frac{\bar{S}_{11} - \bar{S}_{13}}{2}$ $\bar{S}_{13}$ $\frac{\bar{S}_{11} - \bar{S}_{13}}{2}$	Tetragonal	45 D alt	011 110 101	Body-centered $\sqrt{\frac{2}{3}} \le \frac{c}{a} < \sqrt{2}$
$\bar{S}_{23}$ $\bar{0}$ $\bar{0}$	Orthorhombic	50 D deg	011 $0\bar{1}1$ 100	C-centered $\frac{d^2}{4} < a^2; \frac{d^2}{4} = c^2$
$\bar{S}_{23}$ $\bar{0}$ $\frac{\bar{S}_{11}}{2}$	Monoclinic	54 A deg	120 100 001	End-centered $b^2 = c^2 = \frac{d^2}{4}$
$\bar{S}_{23}$ $\bar{0}$ $\bar{S}_{23}$	Monoclinic	55 A deg	101 $\bar{1}01$ 010	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c \quad a = b$
$\bar{S}_{23}$ $\frac{\bar{S}_{11}}{2}$ $\bar{0}$	Monoclinic	54 A deg	102 100 010	End-centered $b^2 = c^2 = \frac{d^2}{4}$
$\bar{S}_{23}$ $\frac{\bar{S}_{11}}{2}$ $\frac{\bar{S}_{11}}{2}$	Orthorhombic	52 B deg	100 111 $0\bar{1}1$	Body-centered $a^2 = \frac{d^2}{4} < b^2 < c^2$ See Note 3
$\bar{S}_{23}$ $\frac{\bar{S}_{11} - \bar{S}_{23}}{2}$ $\frac{\bar{S}_{11} - \bar{S}_{23}}{2}$	Tetragonal	45 D alt	110 101 011	Body-centered $\sqrt{\frac{2}{3}} \le \frac{c}{a} < \sqrt{2}$
$\bar{S}_{23}$ $\bar{S}_{23}$ $\bar{0}$	Monoclinic	55 A deg	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c \quad a = b$

$\bar{S}_{23}$ $\bar{S}_{23}$ $\bar{S}_{23}$	Rhombohedral	49 D std	$1\bar{1}0$ $\bar{1}01$ $\overline{111}$	Transformation results in a hexogonal lattice $-.333 < \cos \alpha_r < 0.0$
$\bar{S}_{23}$ $\bar{S}_{23}$ $\bar{S}_{12}$	Monoclinic	55 A deg	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$
$\bar{S}_{23}$ $\bar{S}_{13}$ $\bar{S}_{23}$	Monoclinic	55 A deg	101 $\bar{1}01$ 010	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$
$\bar{S}_{23}$ $\bar{S}_{13}$ $\bar{S}_{13}$	Monoclinic	55 A deg	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} = c$
$\bar{S}_{23}$ $\bar{S}_{13}$ $(\bar{S}_{11} - \bar{S}_{23} - \bar{S}_{13})$	Orthorhombic	52 A std	101 110 011	Body-centered $\frac{d^2}{4} < a^2 < b^2 < c^2$ See Note 1

Symmetrical Scalars: $S_{11} = S_{22} \neq S_{33}$

Unsymmetrical Scalars: +	Lattice	Niggli Figure	Transformation Matrix	Comments
$\frac{S_{11}}{4}$ $\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$	Orthorhombic	51 B deg	$\bar{1}20$ $\bar{1}02$ 100	Face-centered $a^2 = 3c^2$
$\frac{S_{11}}{2}$ $\frac{S_{11}}{4}$ $\frac{S_{11}}{2}$	Orthorhombic	51 B deg	$2\bar{1}0$ $0\bar{1}2$ 010	Face-centered $a^2 = 3c^2$
$\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$	Rhombohedral	49 B std	100 $\bar{1}10$ $\bar{1}\bar{1}3$	Transformation matrix results in a hexagonal lattice $0.5 < \cos \alpha_r < 1.0$
$\frac{S_{11}}{2}$ $\frac{S_{12}}{2}$ S_{12}	Monoclinic	56 A deg	$0\bar{1}0$ $0\bar{1}2$ 100	End-centered $a^2 = c^2 < \frac{d^2}{4}$
$\frac{S_{11}}{2}$ S_{13} $\frac{S_{11}}{2}$	Monoclinic	57 C deg	$10\bar{1}$ 010 $1\bar{1}1$	Body-centered See Figure, Appendix A Note 6, Appendix B
$\frac{S_{13}}{2}$ S_{13} $\frac{S_{11}}{2}$	Monoclinic	56 A deg	$\bar{1}00$ $\bar{1}20$ 001	End centered $a^2 = \frac{d^2}{4} < c^2$
$\frac{S_{12}}{2}$ $\frac{S_{11}}{2}$ S_{12}	Monoclinic	56 A deg	$\bar{1}00$ $\bar{1}02$ 010	End-centered $a^2 = c^2 < \frac{d^2}{4}$
S_{23} $\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$	Monoclinic	57 C deg	$01\bar{1}$ 100 $\bar{1}11$	Body-centered See Figure, Appendix A Note 6, Appendix B

S_{23} $\frac{S_{23}}{2}$ $\frac{S_{11}}{2}$	Monoclinic	56 A deg	$0\bar{1}0$ $2\bar{1}0$ 001	End-centered $a^2 = \frac{d^2}{4} < c^2$
S_{23} S_{23} 0	Monoclinic	55 A deg	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} < c \quad a = b$
S_{23} S_{23} S_{12}	Monoclinic	55 A std	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(2^2 +c\ ^2)^{\frac{1}{2}} < c$

Symmetrical Scalars: $S_{11} = S_{22} \neq S_{33}$

Unsymmetrical Scalars: -	Lattice	Niggli Figure	Transformation Matrix	Comments
$\bar{0}\ \bar{0}\ \bar{0}$	Tetragonal	45 A std	100 010 001	$\frac{c}{a} > 1.0$
$\bar{0}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Hexagonal	48 A std	100 010 001	$\frac{c}{a} > 1.0$
$\bar{0}\ \bar{0}\ \bar{S}_{12}$	Orthorhombic	50 D std	110 $\bar{1}10$ 001	C - centered $\frac{d^2}{4} < a^2,\ \frac{d^2}{4} < c^2$
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Orthorhombic	50 A deg	100 $\bar{1}0\bar{2}$ 010	C - centered $a^2 = c^2 < \frac{d^2}{4}$
$\bar{0}\ \bar{S}_{13}\ \bar{0}$	Monoclinic	53 A deg	100 010 001	Simple $a = b < c$
$\bar{0}\ \bar{S}_{13}\ \frac{\bar{S}_{11}}{2}$	Monoclinic	54 A deg	210 010 001	End-centered $b^2 = \frac{d^2}{4} < c^2$
$\frac{\bar{S}_{11}}{4}\ \frac{\bar{S}_{11}}{4}\ \frac{\bar{S}_{11}}{2}$	Orthorhombic	51 B deg	$1\bar{1}0$ 112 $\bar{1}\bar{1}0$	Face-centered $a^2 = 3\ c^2$
$\frac{\bar{S}_{11}}{2}\ \bar{0}\ \bar{0}$	Orthorhombic	50 A deg	010 $0\bar{1}\bar{2}$ 100	C - centered $a^2 = c^2 < \frac{d^2}{4}$

$\frac{\bar{S}_{11}}{2}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Tetragonal	45 C std	100 010 112	Body-centered $\frac{c}{a} > \sqrt{2}$
$\frac{\bar{S}_{11}}{2}\ \bar{S}_{13}\ \bar{0}$	Monoclinic	54 A deg	012 010 100	End-centered $b^2 = c^2 < \frac{d^2}{4}$
$\bar{S}_{23}\ \bar{0}\ \bar{0}$	Monoclinic	53 A deg	010 100 001	Simple $a = b < c$
$\bar{S}_{23}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Monoclinic	54 A deg	120 100 001	End-centered $b^2 = \frac{d^2}{4} < c^2$
$\bar{S}_{23}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Monoclinic	54 A deg	102 100 010	End-centered $b^2 = c^2 < \frac{d^2}{4}$
$\bar{S}_{23}\ \bar{S}_{23}\ \bar{0}$	Monoclinic	55 A deg	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} < c \quad a = b$
$\bar{S}_{23}\ \bar{S}_{23}\ (\bar{S}_{11} - 2\,\bar{S}_{23})$	Orthorhombic	51 A std	$1\bar{1}0$ 112 $\bar{1}10$	Face-centered $a^2 < 3\,c^2$
$\bar{S}_{23}\ \bar{S}_{23}\ \bar{S}_{12}$	Monoclinic	55 A std	110 $\bar{1}10$ 001	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} < c$
$\bar{S}_{23}\ \bar{S}_{13}\ \frac{\bar{S}_{11}}{2}$	Monoclinic	57 C deg	101 110 $0\bar{1}\bar{1}$	Body-centered See Figure, Appendix A Note 6, Appendix B
$\bar{S}_{23}\ \bar{S}_{13}\ (\bar{S}_{11} - \bar{S}_{23} - \bar{S}_{13})$	Monoclinic	57 B std	011 110 101	Body-centered See Figure, Appendix A Note 4, Appendix B

Symmetrical Scalars: $S_{11} \neq S_{22} = S_{33}$ Unsymmetrical Scalars: +	Lattice	Niggli Figure	Transformation Matrix	Comments
$0 \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{2}$	Orthorhombic	52 B std	$\bar{1}00$ $\bar{1}11$ $0\bar{1}1$	Body-centered $a^2 < \frac{d^2}{4} < b^2 < c^2$ See Note 2
$0 \quad S_{13} \quad S_{13}$	Monoclinic	55 B deg	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} > c \quad a = b$
$\frac{S_{11}}{4} \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{2}$	Tetragonal	45 E std	$0\bar{1}1$ $1\bar{1}\bar{1}$ 100	$\frac{c}{a} < \sqrt{\frac{2}{3}}$
$\frac{S_{22}}{2} \quad \frac{S_{12}}{2} \quad S_{12}$	Monoclinic	56 B deg	$0\bar{1}0$ $0\bar{1}2$ 100	End-centered $c^2 < a^2 = \frac{d^2}{4}$
$\frac{S_{22}}{2} \quad S_{13} \quad \frac{S_{13}}{2}$	Monoclinic	56 B deg	$00\bar{1}$ $02\bar{1}$ 100	End-centered $c^2 < a^2 = \frac{d^2}{4}$
$\frac{S_{12}}{2} \quad \frac{S_{11}}{2} \quad S_{12}$	Monoclinic	56 A deg	$\bar{1}00$ $\bar{1}02$ 010	End-centered $a^2 < c^2 = \frac{d^2}{4}$
$\frac{S_{13}}{2} \quad S_{13} \quad \frac{S_{11}}{2}$	Monoclinic	56 A deg	$\bar{1}00$ $\bar{1}20$ 001	End-centered $a^2 < c^2 = \frac{d^2}{4}$
$S_{23} \quad \frac{S_{11}}{2} \quad \frac{S_{11}}{2}$	Orthobrhombic	52 B std	$\bar{1}00$ $\bar{1}11$ $0\bar{1}1$	Body-centered $a^2 < \frac{d^2}{4} < b^2 < c^2$ See Note 2
$S_{23} \quad S_{13} \quad S_{13}$	Monoclinic	55 B std	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} > c$

Symmetrical Scalars: $S_{11} \neq S_{22} = S_{33}$

Unsymmetrical Scalars: -	Lattice	Niggli Figure	Transformation Matrix	Comments
$\bar{0}\ \bar{0}\ \bar{0}$	Tetragonal	45 B std	010 001 100	$\frac{c}{a} < 1.0$
$\bar{0}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Orthorhombic	50 A deg	100 $\bar{1}20$ 001	C - centered $a^2 < c^2 = \frac{d^2}{4}$
$\bar{0}\ \bar{0}\ \bar{S}_{12}$	Monoclinic	53 A deg	100 001 010	Simple $a < b = c$
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Orthorhombic	50 A deg	100 $\bar{1}0\bar{2}$ 010	C - centered $a^2 < c^2 = \frac{d^2}{4}$
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \frac{\bar{S}_{11}}{2}$	Orthorhombic	52 B alt	100 111 $0\bar{1}1$	Body-centered $a^2 < \frac{d^2}{4} < b^2 < c^2$ See Note 2
$\bar{0}\ \bar{S}_{13}\ \bar{0}$	Monoclinic	53 A deg	100 010 001	Simple $a < b = c$
$\bar{0}\ \bar{S}_{13}\ \bar{S}_{13}$	Monoclinic	55 B deg	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} > c \quad a = b$
$\frac{\bar{S}_{11}}{2}\ \bar{0}\ \bar{0}$	Hexagonal	48 B std	010 001 100	$\frac{c}{a} < 1.0$

$\frac{\bar{S}_{22}}{2}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Orthorhombic	52 C deg	100 001 $\overline{121}$	Body-centered $a^2 < b^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{22}}{2}\ \bar{0}\ \bar{S}_{12}$	Monoclinic	54 B deg	021 001 100	End-centered $c^2 < b^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{22}}{2}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Orthorhombic	52 C deg	100 010 $\overline{112}$	Body-centered $a^2 < b^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{22}}{2}\ \bar{S}_{13}\ \bar{0}$	Monoclinic	54 B deg	012 010 100	End-centered $c^2 < b^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{22} - \frac{\bar{S}_{11}}{3}}{2}\ \frac{\bar{S}_{11}}{3}\ \frac{\bar{S}_{11}}{3}$	Rhombohedral	49 E std	121 $0\bar{1}1$ 100	**Transformation matrix results in a hexagonal lattice.** $-1.0 < \cos \alpha_r < -.333$
$\frac{\bar{S}_{22} - \bar{S}_{12}}{2}\ \frac{\bar{S}_{11} - \bar{S}_{12}}{2}\ \bar{S}_{12}$	Monoclinic	57 A deg	100 112 010	Body-centered $a^2 < c^2 = \frac{d^2}{4}$
$\frac{\bar{S}_{22} - \bar{S}_{13}}{2}\ \bar{S}_{13}\ \frac{\bar{S}_{11} - \bar{S}_{13}}{2}$	Monoclinic	57 A deg	100 121 001	Body-centered $a^2 < c^2 = \frac{d^2}{4}$
$\bar{S}_{23}\ \bar{0}\ \bar{0}$	Orthorhombic	50 E std	011 $0\bar{1}1$ 100	C - centered $c^2 < \frac{d^2}{4} < a^2$
$\bar{S}_{23}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Monoclinic	54 A deg	120 100 001	End-centered $b^2 < \frac{d^2}{4} = c^2$

$\bar{S}_{23}$ $\frac{\bar{S}_{11}}{2}$ $\bar{0}$	Monoclinic	54 A deg	102 100 010	End-centered $b^2 < \frac{d^2}{4} = c^2$
$\bar{S}_{23}$ $\frac{\bar{S}_{11}}{2}$ $\frac{\bar{S}_{11}}{2}$	Orthorhombic	52 B alt	100 111 $0\bar{1}1$	Body-centered $a^2 < \frac{d^2}{4} < b^2 < c^2$ See Note 2
$\bar{S}_{23}$ $\bar{S}_{13}$ $\bar{S}_{13}$	Monoclinic	55 B std	011 $0\bar{1}1$ 100	End-centered $\frac{1}{2}(a^2 + b^2)^{\frac{1}{2}} > c$

Symmetrical Scalars: $S_{11} \neq S_{22} \neq S_{33}$

Unsymmetrical Scalars: +	Lattice	Niggli Figure	Transformation Matrix	Comments
$\frac{S_{11}}{4}$ $\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$	Orthorhombic	51 B std	$\bar{1}20$ $\bar{1}02$ 100	Face-centered $a^2 > 3\ c^2$
$\frac{S_{22}}{2}$ $\frac{S_{12}}{2}$ S_{12}	Monoclinic	56 B std	$0\bar{1}0$ $0\bar{1}2$ 100	End-centered $c^2 < a^2 < \frac{d^2}{4}$
$\frac{S_{13}}{2}$ S_{13} $\frac{S_{11}}{2}$	Monoclinic	56 C std	$\bar{1}00$ $\bar{1}20$ 001	End-centered $a^2 < \frac{d^2}{4} < c^2$
$\frac{S_{12}}{2}$ $\frac{S_{11}}{2}$ S_{12}	Monoclinic	56 A std	$\bar{1}00$ $\bar{1}02$ 010	End-centered $a^2 < c^2 < \frac{d^2}{4}$
S_{23} $\frac{S_{11}}{2}$ $\frac{S_{11}}{2}$	Monoclinic	57 C std	$01\bar{1}$ 100 $\bar{1}11$	Body-centered See Figure, Appendix A Note 5, Appendix B
S_{23} S_{13} S_{12}	Triclinic	58 A std	100 010 001	None

Symmetrical Scalars: $S_{11} \neq S_{22} \neq S_{33}$

Unsymmetrical Scalars: -	Lattice	Niggli Figure	Transformation Matrix	Comments
$\bar{0}\ \bar{0}\ \bar{0}$	Orthorhombic	50 C std	100 010 001	Simple $a^2 < b^2 < c^2$
$\bar{0}\ \bar{0}\ \frac{\bar{S}_{11}}{2}$	Orthorhombic	50 B std	100 $\bar{1}\bar{2}0$ 001	C - centered $a^2 < \frac{d^2}{4} < c^2$
$\bar{0}\ \bar{0}\ \bar{S}_{12}$	Monoclinic	53 C std	100 001 010	Simple $a < c < b$
$\bar{0}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Orthorhombic	50 A std	100 $\bar{1}0\bar{2}$ 010	C - centered $a^2 < c^2 < \frac{d^2}{4}$
$\bar{0}\ \bar{S}_{13}\ \bar{0}$	Monoclinic	53 A std	100 010 001	Simple $a < b < c$
$\frac{\bar{S}_{22}}{2}\ \bar{0}\ \bar{0}$	Orthorhombic	50 F std	010 $0\bar{1}\bar{2}$ 100	C - centered $c^2 < a^2 < \frac{d^2}{4}$
$\frac{\bar{S}_{22}}{2}\ \frac{\bar{S}_{11}}{2}\ \bar{0}$	Orthorhombic	52 C std	100 010 $\bar{1}\bar{1}\bar{2}$	Body-centered $a^2 < b^2 < \frac{d^2}{4} < c^2$
$\frac{\bar{S}_{22}}{2}\ \bar{S}_{13}\ \bar{0}$	Monoclinic	54 B std	012 010 100	End-centered $c^2 < b^2 < \frac{d^2}{4}$

$\frac{\bar{S}_{22}-\bar{S}_{12}}{2}$ $\frac{\bar{S}_{11}-\bar{S}_{12}}{2}$ $\bar{S}_{12}$	Monoclinic	57 A std	100 112 010	Body-centered $a^2 < c^2 < \frac{d^2}{4}$
$\bar{S}_{23}$ $\bar{0}$ $\bar{0}$	Monoclinic	53 B std	010 100 001	Simple $b < a < c$
$\bar{S}_{23}$ $\bar{0}$ $\frac{\bar{S}_{11}}{2}$	Monoclinic	54 A std	120 100 001	End-centered $b^2 < \frac{d^2}{4} < c^2$
$\bar{S}_{23}$ $\frac{\bar{S}_{11}}{2}$ $\bar{0}$	Monoclinic	54 C std	102 100 010	End-centered $b^2 < c^2 < \frac{d^2}{4}$
$\bar{S}_{23}$ $\frac{\bar{S}_{11}}{2}$ $\frac{\bar{S}_{11}}{2}$	Monoclinic	57 C alt	111 100 $01\bar{1}$	Body-centered See Figure, Appendix A Note 5, Appendix B
$\bar{S}_{23}$ $\bar{S}_{13}$ $\bar{S}_{12}$	Triclinic	58 B std	100 010 001	None

Note 1: For 52A, eee, it is possible for one unit cell to yield six reduced cells. This is accomplished by a cyclic permutation of the unsymmetrical scalars, which, in turn, results in a cyclic permutation of the orthorhombic unit cell axes. For all these cells, however, the sum of the unsymmetrical scalars is equal to S_{11} and the final choice of the individual a, b, c axes is left to the investigator.

Note 2: For 52B, eff, it is possible for one unit cell to have two different values for S_{23}. These correspond to an interchange of the orthorhombic b and c axes, and the final choice is left to the investigator. The algebraic signs for the two values of S_{23} may be either (+, +) or (+, -). Consequently, it is possible, when the algebraic sign changes from + to -, for S_{23} to have the value $\pm$ 0.0.

Note 3: For 52B, eee, if all diagonal vectors are chosen, then this case is identical with the general case 52A. If an axial vector plus diagonal vectors are chosen, then all unsymmetrical scalars are permuted. The algebraic signs of S_{23} (or S_{13} or S_{12}) may be again in the general case (+, +) or (+, -). For S_{23} (or S_{13} or S_{12}) = + 0.0, an alternative representation for the face-centered cubic is obtained. For S_{23} (or S_{13} or S_{12}) = -0.0, the tetragonal representation of the face-centered cubic is obtained.

Note 4: For 57B, eef, an interchange in positions for the values $\bar{S}_{23}$ and $\bar{S}_{13}$ is to be expected. This results in merely an interchange of the final a and c axes. The correct β angle is calculated in either case. The sum of unsymmetrical scalars equals S_{11}.

Note 5: For 57C, efg, it is possible that a reduced cell of the variety $\bar{S}_{23}$, 1/2 $\bar{S}_{11}$, 1/2 $\bar{S}_{11}$ may exist. This cell is designated as an alternative standard representation.

Note 6: For 57C, eef, two different positive values for S_{23} exist. Use of one or the other causes only an interchange of the unit cell a and c axes. An interchange of S_{23} and 1/2 S_{11} is also to be expected. In addition there exists a reduced cell having the characteristics $\bar{S}_{23}$ $\bar{S}_{13}$ $\frac{\bar{S}_{11}}{2}$. An interchange of $\bar{S}_{23}$ and $\bar{S}_{13}$ values is to be expected and results in an interchange of the a and c axes in the transformed unit cell.

Appendix C.

An alternative method leading to the derivation of Niggli matrices

Niggli derived his 41 standard general reduced cells by applying Eisenstein's (1851) theory of reduced ternary quadratic forms to the equation for determining the absolute length of any vector, $\underset{\sim}{t}$, in any lattice. This equation is

$$
\begin{aligned}
|\underline{t}|^2 = U^2\underline{a}^2 + V^2\underline{b}^2 + W^2\underline{c}^2 &+ 2\,U\,V\,\underline{ab}\cos\gamma \\
&+ 2\,U\,W\,\underline{ac}\cos\beta \\
&+ 2\,V\,W\,\underline{bc}\cos\alpha
\end{aligned}
$$

where $\underline{a}$, $\underline{b}$, $\underline{c}$, α, β, and γ are the cell constants and U, V, W are integers. The above equation may be identified with the following equation of Eisenstein

$$
\begin{aligned}
f = x^2a + y^2b + z^2c &+ 2\,x\,y\,t \\
&+ 2\,x\,z\,s \\
&+ 2\,y\,z\,r
\end{aligned}
$$

Subject to a series of rather remarkable conditions, Eisenstein questions may be <u>reduced</u>, i.e., a unique solution may be found. If two or more Eisenstein equations are to be classed as equivalent, one merely need compare their reduced forms. If the reduced forms are equivalent, the original equations are equivalent.

The Eisenstein conditions applicable to the crystallographic equation given above are:

If (1), $\underline{a}\ \underline{b}\cos\gamma$, $\underline{a}\ \underline{c}\cos\beta$, $\underline{b}\ \underline{c}\cos\alpha$ are all positive or all negative;

then (2), $\underline{a}^2 \leq \underline{b}^2 \leq \underline{c}^2$, $[\underline{a}^2 + \underline{b}^2 + 2\,\underline{b}\ \underline{c}\cos\alpha + 2\,\underline{a}\ \underline{c}\cos\beta + 2\,\underline{a}\ \underline{b}\cos\gamma \geq 0]$;

and (3), $\underline{a}^2 \geq |\,2\,\underline{a}\ \underline{c}\cos\beta\,|$, $\underline{a}^2 \geq |\,2\,\underline{a}\ \underline{b}\cos\gamma\,|$, $\underline{b}^2 \geq |\,2\,\underline{b}\ \underline{c}\cos\alpha|$;

and (4), if $\underline{a}^2 = \underline{b}^2$, $|\,\underline{b}\ \underline{c}\cos\alpha\,| \leq |\,\underline{a}\ \underline{c}\cos\beta\,|$;

if $\underline{b}^2 = \underline{c}^2$, $|\,\underline{a}\ \underline{c}\cos\beta\,| \leq |\,\underline{a}\ \underline{b}\cos\gamma\,|$;

if $[\underline{a}^2 + \underline{b}^2 + 2\,\underline{b}\ \underline{c}\cos\alpha + 2\,\underline{a}\ \underline{c}\cos\beta + 2\,\underline{a}\ \underline{b}\cos\gamma = 0$,

$\underline{a}^2 + 2\,\underline{a}\ \underline{c}\cos\beta + \underline{a}\ \underline{b}\cos\gamma \leq 0]$.

However, (5), for $\underline{a}\ \underline{b}\cos\gamma$, $\underline{a}\ \underline{c}\cos\beta$, $\underline{b}\ \underline{c}\cos\alpha \leq 0$;

if $\underline{a}^2 = -\,2\,\underline{a}\ \underline{b}\cos\gamma$, then $\underline{a}\ \underline{c}\cos\beta = 0$;

if $\underline{a}^2 = -\,2\,\underline{a}\ \underline{c}\cos\beta$, then $\underline{a}\ \underline{b}\cos\gamma = 0$;

if $\underline{b}^2 = -\,2\,\underline{b}\ \underline{c}\cos\alpha$, then $\underline{a}\ \underline{b}\cos\gamma = 0$;

Also, (6), for $\underline{a}\ \underline{b}\cos\gamma$, $\underline{a}\ \underline{c}\cos\beta$, $\underline{b}\ \underline{c}\cos\alpha > 0$;

if $\underline{a}^2 = 2\,\underline{a}\ \underline{b}\cos\gamma$, then $\underline{a}\ \underline{c}\cos\beta \leq 2\,\underline{b}\ \underline{c}\cos\alpha$;

if $\underline{a}^2 = 2\,\underline{a}\ \underline{c}\cos\beta$, then $\underline{a}\ \underline{b}\cos\gamma \leq 2\,\underline{b}\ \underline{c}\cos\alpha$;

if $\underline{b}^2 = 2\,\underline{b}\ \underline{c}\cos\alpha$, then $\underline{a}\ \underline{b}\cos\gamma \leq 2\,\underline{a}\ \underline{c}\cos\beta$.

The conditions in brackets [ ] are omitted unless $\underline{a}\ \underline{b}\cos\gamma$, $\underline{a}\ \underline{b}\cos\beta$, $\underline{b}\ \underline{c}\cos\alpha$ are all < 0.

According to the definition of a lattice any lattice point may be reached from any other lattice point by appropriate translation of the vectors (or fractions of the vectors) chosen to describe the edges of the unit cell. It follows then, that the vector distance from an origin to any given lattice point may be found for any of the infinite number of unit cells that may be defined.

The Eisenstein conditions given above imply that any lattice and any vector distance may be examined by the following procedure:

In a given lattice let a unit cell be chosen. Let the cell be subjected to the Eisenstein conditions. If the cell passes all the criteria implied by the conditions, it is said to be Eisenstein reduced and may represent a unique solution. If the cell chosen does not pass the conditions it is not Eisenstein reduced and the implication is that another cell must be chosen if a unique solution is desired.

The application of Eisenstein conditions to several types of cells is illustrated below.

Example 1. For a simple cubic cell (Fig. 44A, Appendix A) let the cell chosen be:

$\underline{a} = \underline{a}$ for which $\cos\alpha = 0$ and $\underline{a}\ \underline{b} \cos\gamma = 0$

$\underline{b} = \underline{a}$ $\quad\cos\beta = 0 \quad \underline{a}\ \underline{c} \cos\beta = 0$

$\underline{c} = \underline{a}$ $\quad\cos\gamma = 0 \quad \underline{b}\ \underline{c} \cos\alpha = 0$

Then, Condition (1) is satisfied; +, +, +.

Condition (2) is satisfied; $\underline{a}^2 = \underline{a}^2 = \underline{a}^2$.

Condition (3) is satisfied; $\underline{a}^2 > 0$, $\underline{a}^2 > 0$, $\underline{a}^2 > 0$.

Condition (4) is satisfied; $\underline{a}^2 = \underline{a}^2$, $0 = 0$;

$$\underline{a}^2 = \underline{a}^2,\ 0 = 0.$$

Condition (5) is satisfied; 0, 0, 0, = 0; remainder is not applicable.

Condition (6) is not applicable.

Since the chosen cell passes all the criteria implied by the conditions, the cell is Eisenstein reduced.

Example 2a. For a body-centered cubic cell (Fig. 44B, Appendix A) let the cell chosen be:

$\underline{a} = 1/2\ \underline{a}\sqrt{3}$ (1/2 diagonal of cell) for which $\cos\alpha = 1/\sqrt{2}$

$\underline{b} = \underline{a}$ (cell edge) $\cos\beta = \sqrt{2}/\sqrt{3}$

$\underline{c} = \underline{a}\sqrt{2}$ (diagonal of cell face) $\cos\gamma = 1/\sqrt{3}$

and $\underline{a}\ \underline{b}\cos\gamma = 1/2\ \underline{a}^2$

$\underline{a}\ \underline{c}\cos\beta = \underline{a}^2$

$\underline{b}\ \underline{c}\cos\alpha = \underline{a}^2$

Then, Condition (1) is satisfied; +, +, +.

Condition (2) is satisfied; $3/4\ \underline{a}^2 < \underline{a}^2 < 2\ \underline{a}^2$.

Condition (3) is not satisfied; $3/4\ \underline{a}^2 \not\geq |2\ \underline{a}^2|$.

Since the chosen cell is not reduced, a new cell should be chosen if a unique cell is desired.

Example 2b. For a body-centered cubic cell (Fig. 44B, Appendix A) let the cell chosen be:

$\underline{a} = 1/2\ \underline{a}\sqrt{3}$ for which $\cos\alpha = -1/3$ and $\underline{a}\ \underline{b}\cos\gamma = -1/4\ \underline{a}^2$

$\underline{b} = 1/2\ \underline{a}\sqrt{3}$ $\cos\beta = -1/3$ $\underline{a}\ \underline{c}\cos\beta = -1/4\ \underline{a}^2$

$\underline{c} = 1/2\ \underline{a}\sqrt{3}$ $\cos\gamma = -1/3$ $\underline{b}\ \underline{c}\cos\alpha = -1/4\ \underline{a}^2$

Then, Condition (1) is satisfied; -, -, -.

Condition (2) is satisfied; $3/4\ \underline{a}^2 = 3/4\ \underline{a}^2 = 3/4\ \underline{a}^2$,

$[\ 3/4\ \underline{a}^2 + 3/4\ \underline{a}^2 - 2/4\ \underline{a}^2 - 2/4\ \underline{a}^2 - 2/4\ \underline{a}^2 = 0]$.

Condition (3) is satisfied; $3/4\ \underline{a}^2 > 2/4\ \underline{a}^2$, $3/4\ \underline{a}^2 > 2/4\ \underline{a}^2$,

$3/4\ \underline{a}^2 > 2/4\ \underline{a}^2$.

Condition (4) is satisfied; $3/4\ \underline{a}^2 = 3/4\ \underline{a}^2$, $1/4\ \underline{a}^2 = 1/4\ \underline{a}^2$,

$3/4\ \underline{a}^2 = 3/4\ \underline{a}^2$, $1/4\ \underline{a}^2 = 1/4\ \underline{a}^2$,

$[3/4\ \underline{a}^2 + 3/4\ \underline{a}^2 - 2/4\ \underline{a}^2 - 2/4\ \underline{a}^2 - 2/4\ \underline{a}^2 = 0$,

$3/4\ \underline{a}^2 - 2/4\ \underline{a}^2 - 1/4\ \underline{a}^2 = 0]$.

Condition (5) is satisfied; -, -, -; remainder is not applicable.

Condition (6) is not applicable.

Since the chosen cell passes all the relevant tests, it is Eisenstein reduced.

Example 3a. For a face-centered cubic cell (Fig. 44C, appendix A) let the cell chosen be:

$\underline{a} = 1/2\ \underline{a}\sqrt{2}$ for which $\cos\alpha = 1/2$ and $\underline{a}\ \underline{b}\cos\gamma = 1/4\ \underline{a}^2$

$\underline{b} = 1/2\ \underline{a}\sqrt{2}$ $\cos\beta = 1/2$ $\underline{a}\ \underline{c}\cos\beta = 1/4\ \underline{a}^2$

$\underline{c} = 1/2\ \underline{a}\sqrt{2}$ $\cos\gamma = 1/2$ $\underline{b}\ \underline{c}\cos\alpha = 1/4\ \underline{a}^2$

Then, Condition (1) is satisfied; +, +, +.

Condition (2) is satisfied; $1/2\ \underline{a}^2 = 1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$.

Condition (3) is satisfied; $1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, $1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$,
$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$.

Condition (4) is satisfied; $1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, $1/4\ \underline{a}^2 = 1/4\ \underline{a}^2$,
$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, $1/4\ \underline{a}^2 = 1/4\ \underline{a}^2$.

Condition (5) is not applicable.

Condition (6) is satisfied; +, +, +
$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, and $1/4\ \underline{a}^2 < 1/2\ \underline{a}^2$,
$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, and $1/4\ \underline{a}^2 < 1/2\ \underline{a}^2$,
$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, and $1/4\ \underline{a}^2 < 1/2\ \underline{a}^2$.

The chosen cell is thus Eisenstein reduced.

Example 3b. For a face-centered cubic cell (Fig. 44C, Appendix A) let the cell chosen be:

$\underline{a} = 1/2\ \underline{a}\sqrt{2}$ for which $\cos\alpha = -0$ and $\underline{a}\ \underline{b}\cos\gamma = -1/4\ \underline{a}^2$,
$\underline{b} = 1/2\ \underline{a}\sqrt{2}$ $\qquad \cos\beta = -1/2 \qquad \underline{a}\ \underline{c}\cos\beta = -1/4\ \underline{a}^2$,
$\underline{c} = 1/2\ \underline{a}\sqrt{2}$ $\qquad \cos\gamma = -1/2 \qquad \underline{b}\ \underline{c}\cos\alpha = -0$.

Then, Condition (1) is satisfied; -, -, -.

Condition (2) is satisfied; $1/2\ \underline{a}^2 = 1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$,
$[\ 1/2\ \underline{a}^2 + 1/2\ \underline{a}^2 - 0 - 1/2\ \underline{a}^2 - 1/2\ \underline{a}^2 = 0]$.

Condition (3) is satisfied; $1/2\ \underline{a}^2 = |-1/2\ \underline{a}^2|$, $1/2\ \underline{a}^2 = |-1/2\ \underline{a}^2|$,
$1/2\ \underline{a}^2 > |-0|$.

Condition (4) is satisfied; $1/2\ \underline{a}^2 = 1/2\ \underline{a}^2$, $|-0|<|-1/4\ \underline{a}^2|$,

$$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2,\ |-1/4\ \underline{a}^2| = |-1/4\ \underline{a}^2|,$$

$$[1/2\ \underline{a}^2 + 1/2\ \underline{a}^2 - 0 - 1/2\ \underline{a}^2 - 1/2\ \underline{a}^2 = 0,$$

$$1/2\ \underline{a}^2 - 1/2\ \underline{a}^2 - 1/4\ \underline{a}^2 < 0\ ].$$

Condition (5) is not satisfied; -, -, -

$$1/2\ \underline{a}^2 = 1/2\ \underline{a}^2, \text{but} - 1/4\ \underline{a}^2 \not> 0.$$

Therefore the chosen cell is not Eisenstein reduced.

Jones (1935) writes that for any given point lattice an Eisenstein reduction (Parenthetical insertions by Roof)

> "amounts to picking a coordinate system (i.e., a unit cell) as follows: choose any point O of the lattice as the origin, call A one of the points of the lattice closest to O, draw the X axis along OA, choose as B one of the points as close to O (X, i.e., the X axis) as any point of the lattice not on the X axis and draw the Y axis along OB, choose as C one of the points as close to O as any point of the lattice not in the XY plane and draw the Z axis along OC."

A systematic application of this recipe to the point lattices having various generalized dimensional configurations will yield the 41 Niggli reduced cells. The addition of the expression (X, i.e., the X axis), to the above definition is important, as it was shown in Example 3b that a lattice point may be chosen "as close to O as any point of the lattice not on the X axis," which does not yield an Eisenstein reduction. On the other hand, in Example 3a an Eisenstein reduction is obtained if the lattice point chosen is the one closest to the OX line, i.e., the X axis.

The cell chosen in 3b, while it is composed of a set of three shortest noncoplanar vectors having the cosines of the interaxial angles all negative and may therefore be classed as reduced, is not Eisenstein reduced. It is actually a very special case that would occur in the body-centered tetragonal lattice (Fig. 45C, Appendix A) when the ratio $\underline{c}/\underline{a} = \sqrt{2}$. In this case the Eisenstein reduced form is the reduced cell given in Example 3a for the face-centered cubic lattice.

The 41 Niggli matrices are all Eisenstein reduced. It does not necessarily follow that special or degenerate representations of these matrices will yield cells that are themselves Eisenstein reduced. A hexagonal lattice having $\underline{c}/\underline{a} = 1.0$ generates a special Niggli representation, and the reduced cell (in standard orientation) is also Eisenstein reduced. However, a body-centered tetragonal lattice with $\underline{c}/\underline{a} = \sqrt{2}$ also generates a special Niggli representation but the reduced cell (in standard orientation) is not Eisenstein reduced.